

10/539372

=> s l1

SAMPLE SEARCH INITIATED 11:59:13 FILE 'REGISTRY'

SAMPLE SCREEN SEARCH COMPLETED - 96966 TO ITERATE

2.1% PROCESSED 2000 ITERATIONS

0 ANSWERS

INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)

SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE \*\*INCOMPLETE\*\*

BATCH \*\*INCOMPLETE\*\*

PROJECTED ITERATIONS: 1920831 TO 1957809

PROJECTED ANSWERS: 0 TO 0

L2 0 SEA SSS SAM L1

=>

Uploading C:\Documents and Settings\EBernhardt\My  
Documents\Stnexp\Queries\10539372-2.str



chain nodes :

1 2 3 4 5 6 7 8 9 11 12 13 15 44

ring nodes :

16 17 18 19 20 21 22 23 24 25 26 27 28 29 30 31 32 33 34 35 36  
37 38

ring/chain nodes :

14

chain bonds :

1-11 1-9 1-8 1-44 2-3 2-11 3-4 3-12 3-13 4-5 4-14 5-6 6-7 6-15

10/539372

ring bonds :  
16-17 16-20 17-18 18-19 19-20 21-22 21-26 22-23 23-24 24-25 25-26 27-28  
27-32 28-29 29-30 30-31 31-32 33-34 33-38 34-35 35-36 36-37 37-38  
exact/norm bonds :  
1-11 1-44 2-3 2-11 4-5 5-6 6-7 6-15 16-17 16-20 17-18 18-19 19-20  
21-22 21-26 22-23 23-24 24-25 25-26 27-28 27-32 28-29 29-30 30-31 31-32  
33-34 33-38 34-35 35-36 36-37 37-38  
exact bonds :  
1-9 1-8 3-4 3-12 3-13 4-14

G1:C,O,N

G2:[\*1],[\*2],[\*3],[\*4]

Match level :  
1:CLASS 2:CLASS 3:CLASS 4:CLASS 5:CLASS 6:CLASS 7:CLASS 8:CLASS 9:CLASS  
11:CLASS 12:CLASS 13:CLASS 14:CLASS 15:Atom 16:Atom 17:Atom 18:Atom 19:Atom  
20:Atom 21:Atom 22:Atom 23:Atom 24:Atom 25:Atom 26:Atom 27:Atom 28:Atom  
29:Atom 30:Atom 31:Atom 32:Atom 33:Atom 34:Atom 35:Atom 36:Atom 37:Atom  
38:Atom 44:CLASS  
Generic attributes :  
15:  
Saturation : Unsaturated

L3 STRUCTURE UPLOADED

=> s 13

SAMPLE SEARCH INITIATED 12:07:03 FILE 'REGISTRY'  
SAMPLE SCREEN SEARCH COMPLETED - 43107 TO ITERATE

4.6% PROCESSED 2000 ITERATIONS 0 ANSWERS  
INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)  
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE \*\*COMPLETE\*\*  
BATCH \*\*COMPLETE\*\*  
PROJECTED ITERATIONS: 849741 TO 874539  
PROJECTED ANSWERS: 0 TO 0

L4 0 SEA SSS SAM L3

=> s 13 sss full

FULL SEARCH INITIATED 12:07:14 FILE 'REGISTRY'  
FULL SCREEN SEARCH COMPLETED - 862126 TO ITERATE

95.8% PROCESSED 825571 ITERATIONS 84 ANSWERS  
100.0% PROCESSED 862126 ITERATIONS 86 ANSWERS  
SEARCH TIME: 00.00.24

L5 86 SEA SSS FUL L3

10/539372

=> file caplus  
COST IN U.S. DOLLARS

SINCE FILE	TOTAL
ENTRY	SESSION
178.40	178.61

FULL ESTIMATED COST

FILE 'CAPLUS' ENTERED AT 12:07:46 ON 27 DEC 2007  
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FILE COVERS 1907 - 27 Dec 2007 VOL 147 ISS 26  
FILE LAST UPDATED: 26 Dec 2007 (20071226/ED)

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=> s 15

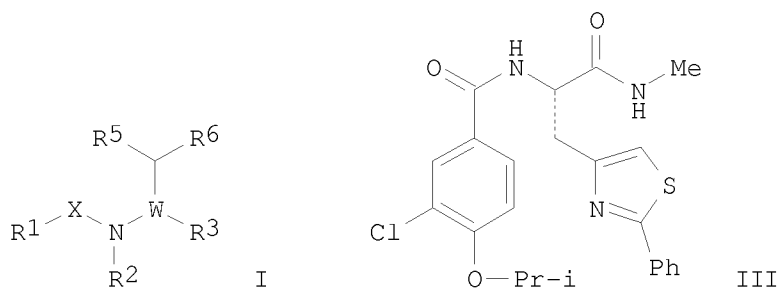
L6 22 L5

=> d 16 1-22 bib abs hitstr

L6 ANSWER 1 OF 22 CAPLUS COPYRIGHT 2007 ACS on STN  
AN 2007:705111 CAPLUS  
DN 147:143660  
TI Preparation of 3-chloro-4-isopropoxybenzamide and 3-cyano-4-isopropoxybenzamide derivatives as inhibitors of mitotic kinesins  
IN Qian, Xiangping; Ashcraft, Luke W.; Wang, Jianchao; Yao, Bing; Jiang, Hong; Bergnes, Gustave; Morgan, Bradley P.; Morgans, David J.; Dhanak, Dashyant; Knight, Steven D.; Adams, Nicholas D.; Parrish, Cynthia A.; Duffy, Kevin J.; Fitch, Duke; Tedesco, Rosanna  
PA USA  
SO U.S. Pat. Appl. Publ., 171pp., Cont.-in-part of U.S. Ser. No. 271,147. CODEN: USXXCO  
DT Patent  
LA English  
FAN.CNT 4

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
	-----	----	-----	-----	-----
PI	US 2007149516	A1	20070628	US 2006-598250	20061108
	US 2006247289	A1	20061102	US 2005-271147	20051109
PRAI	US 2005-271147	A2	20051109		
	US 2004-569510P	P	20040506		
	US 2005-121709	A2	20050503		
	US 2005-124608	A2	20050506		

OS MARPAT 147:143660  
GI



AB The title compds. [I; R1 = 3-halo-4-((R)-1,1,1-trifluoropropan-2-yloxy)phenyl, 3-cyano-4-((R)-1,1,1-trifluoropropan-2-yloxy)phenyl, 3-halo-4-isopropylaminophenyl, 3-cyano-4-isopropylaminophenyl, 3-halo-4-((R)-1,1,1-trifluoropropan-2-ylamino)phenyl, 3-cyano-4-((R)-1,1,1-trifluoropropan-2-ylamino)phenyl; X = CO, SO<sub>2</sub>; R2 = H, (un)substituted lower alkyl; W = CR<sub>4</sub>, CH<sub>2</sub>CR<sub>4</sub>, N; R3 = COR<sub>7</sub>, H, each (un)substituted substituted alkyl, heterocycloalkyl, heteroaryl, or aryl, cyano, sulfonyl; R4 = H, (un)substituted alkyl; R5 = H, HO, each (un)substituted amino, cycloalkyl, heterocycloalkyl, heteroaryl, or lower alkyl; R6 = H, CONH<sub>2</sub>, (un)substituted alkyl, alkoxy, aryloxy, heteroaryloxy, alkoxycarbonyl, aryl, heteroaryl, cycloalkyl, or heterocycloalkyl; R7 = HO, each (un)substituted lower alkyl, aryl, amino, aralkoxy, or alkoxy; provided that if W is N, then R5 is not hydroxy or (un)substituted amino, and R6 is not optionally substituted alkoxy, optionally substituted aralkoxy, optionally substituted heteroaralkoxy, or optionally substituted amino] are prepared (1R)-1-(methoxycarbonylamino)-1-[4-[4-[(2S)-2-[[[4-((1R)-2,2,2-trifluoroisopropyl)oxy]-3-chlorophenyl]carbonyl]amino]-4-hydroxybutyl]phenyl]-1-ethylimidazol-2-yl]ethane. These compds. including N-benzoyl-amino alcs., N-benzoyl-amino acid amide, N-benzoylsemicarbazide, and N-benzoyl-diamine derivs. are inhibitors of one or more mitotic kinesins and are useful in the treatment of cellular proliferative diseases, for example cancer, hyperplasias, restenosis, cardiac hypertrophy, immune disorders, fungal disorders, and inflammation by modulating the activity of one or more mitotic kinesins. Thus, cyclocondensation of (2S)-2-(tert-butoxycarbonylamino)-5-bromo-4-oxopentanoic acid Me ester with thiobenzamide in the presence of diisopropylethylamine in methanol under refluxing for 24 h gave (2S)-2-(tert-butoxycarbonylamino)-3-(2-phenylthiazol-4-yl)propanoic acid which was treated with CF<sub>3</sub>CO<sub>2</sub>H in CH<sub>2</sub>Cl<sub>2</sub> at room temperature for 10 min to give (2S)-2-amino-3-(2-phenylthiazol-4-yl)propanoic acid (II). II was condensed with 3-chloro-4-isopropoxybenzoic acid pentafluorophenyl ester in the presence of diisopropylethylamine in DMF at room temperature to give (2S)-N-methyl-2-[(3-chloro-4-isopropoxybenzoyl)amino]-3-(2-phenylthiazol-4-yl)propanamide (III). Many of the compds. I showed GI<sub>50</sub> (50% growth inhibition concentration) of ≤10 μM against human ovarian tumor cells Skov-3.

IT 943297-47-0P, N-[(2S)-2-[[[3-Chloro-4-(1-methylethoxy)phenyl]carbonyl]amino]-3-[4-[8-(1-hydroxyethyl)-4-

hydroimidazo[1,2-a]pyridin-2-yl]phenyl]propyl]-2-(pyrrolidin-1-yl)acetamide

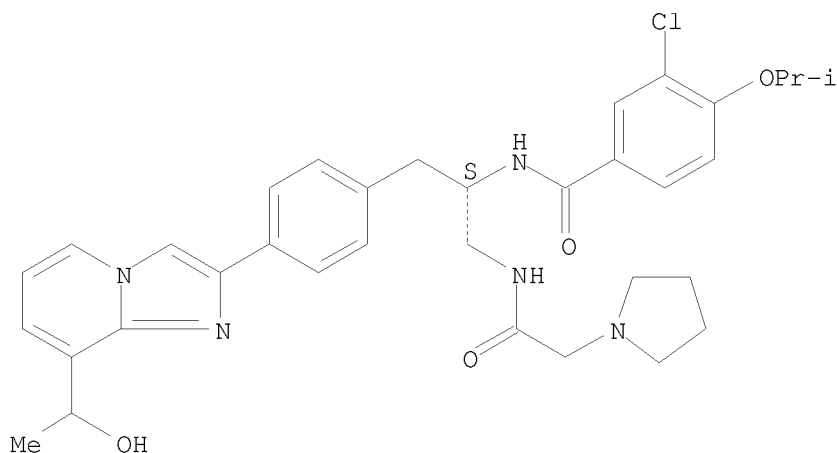
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(preparation of N-benzoyl amino alcs., N-benzoyl-amino acid, N-benzoylsemicarbazide derivs. as inhibitors of mitotic kinesins)

RN 943297-47-0 CAPLUS

CN 1-Pyrrolidineacetamide, N-[(2S)-2-[[3-chloro-4-(1-methylethoxy)benzoyl]amino]-3-[4-[8-(1-hydroxyethyl)imidazo[1,2-a]pyridin-2-yl]phenyl]propyl]- (CA INDEX NAME)

Absolute stereochemistry.



L6 ANSWER 2 OF 22 CAPLUS COPYRIGHT 2007 ACS on STN

AN 2004:863107 CAPLUS

DN 142:48476

TI Nocathiacin I analogues: synthesis, in vitro and in vivo biological activity of novel semi-synthetic thiazolyl peptide antibiotics

AU Naidu, B. Narasimulu; Sorenson, Margaret E.; Zhang, Yunhui; Kim, Oak K.; Matiskella, John D.; Wichtowski, John A.; Connolly, Timothy P.; Li, Wenying; Lam, Kin S.; Bronson, Joanne J.; Pucci, Michael J.; Clark, Junius M.; Ueda, Yasutsugu

CS The Bristol-Myers Squibb Pharmaceutical Research Institute, Wallingford, CT, 06492, USA

SO Bioorganic & Medicinal Chemistry Letters (2004), 14(22), 5573-5577

CODEN: BMCLE8; ISSN: 0960-894X

PB Elsevier B.V.

DT Journal

LA English

OS CASREACT 142:48476

AB Several nocathiacin I analogs were synthesized and evaluated for their antibacterial activity. Most of these semi-synthetic analogs retained very good in vitro and in vivo antibacterial activity of nocathiacin I.

IT 807342-65-0P 807342-68-3P

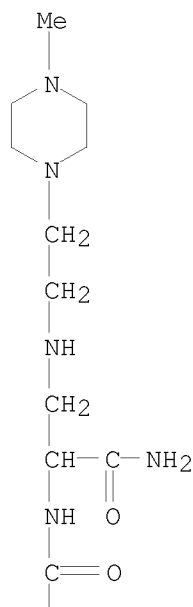
RL: PAC (Pharmacological activity); PRP (Properties); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(synthesis and in vitro and in vivo biol. activity of novel  
semi-synthetic thiazolyl peptide antibiotics nocathiacin I analogs in  
relation to aqueous solubility)

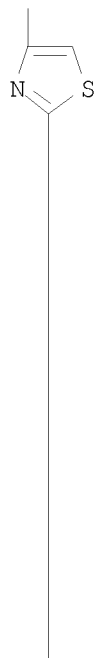
RN 807342-65-0 CAPLUS

CN 4-Thiazolecarboxamide, N-[2-amino-1-[[[2-(4-methyl-1-  
piperazinyl)ethyl]amino]methyl]-2-oxoethyl]-2-[(11S,14E,21S,22S,33S,49S)-  
9,10,11,12,13,14,19,20,21,22,29,30,32,33-tetradecahydro-3,29-dihydroxy-11-  
[(1R)-1-hydroxyethyl]-14-(1-methoxyethylidene)-9,12,19,30,40,48-hexaoxo-49-  
[[2,4,6-trideoxy-4-(dimethylamino)-3-C-methyl- $\alpha$ -L-lyxo-  
hexopyranosyl]oxy]-22,25-(ethanoxymethano)-8,5:18,15:37,34-trinitrilo-  
21,33-([2,4]-endo-thiazolomethanimino)-5H,15H,24H,34H-  
pyrido[3',2':20,21][1,28,8,18,24,4,11,14]dioxatrithiatriazacyclodotriacont  
ino[30,31-b]indol-2-yl]- (9CI) (CA INDEX NAME)

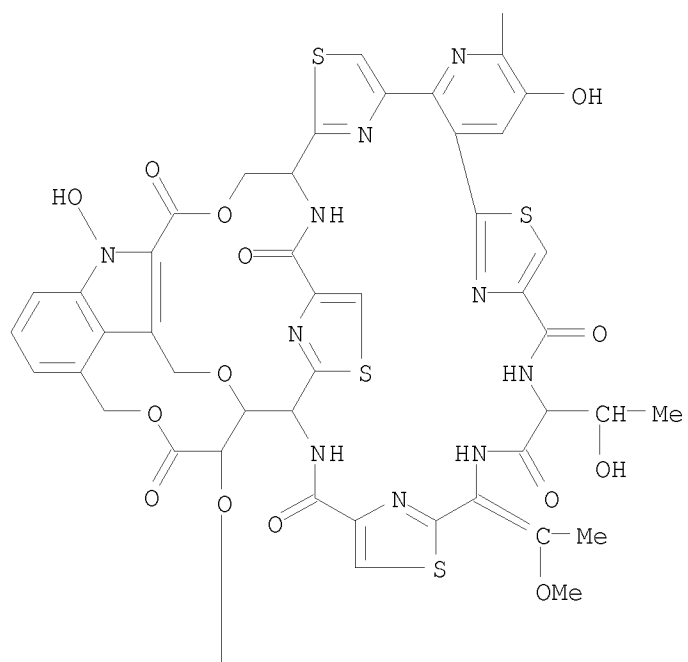
PAGE 1-A



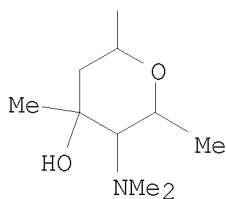
PAGE 2-A



PAGE 3-A

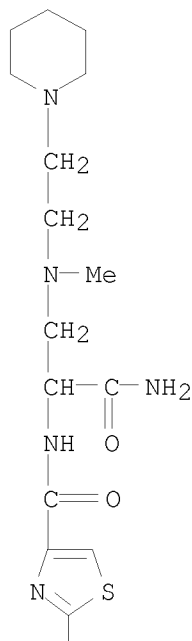


PAGE 4-A

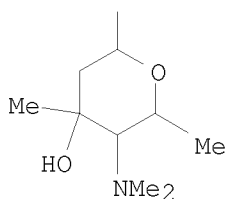
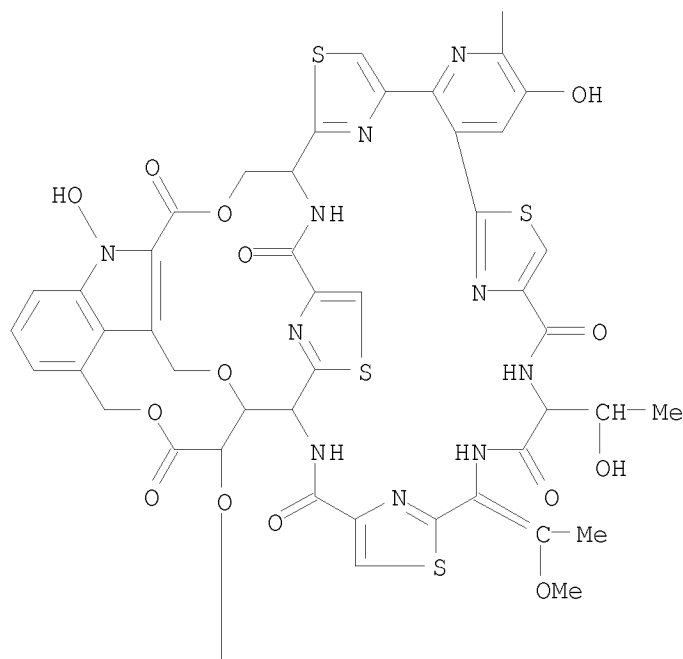


RN 807342-68-3 CAPLUS  
 CN 4-Thiazolecarboxamide, N-[2-amino-1-[[methyl[2-(1-piperidinyl)ethyl]amino]methyl]-2-oxoethyl]-2-[(11S,14E,21S,22S,33S,49S)-9,10,11,12,13,14,19,20,21,22,29,30,32,33-tetradecahydro-3,29-dihydroxy-11-[(1R)-1-hydroxyethyl]-14-(1-methoxyethylidene)-9,12,19,30,40,48-hexaoxo-49-[[2,4,6-trideoxy-4-(dimethylamino)-3-C-methyl- $\alpha$ -L-lyxo-hexopyranosyl]oxy]-22,25-(ethanoxymethano)-8,5:18,15:37,34-trinitrilo-21,33-([2,4]-endo-thiazolomethanimino)-5H,15H,24H,34H-pyrido[3',2':20,21][1,28,8,18,24,4,11,14]dioxatrithiatriazacyclodotriacontino[30,31-b]indol-2-yl]- (9CI) (CA INDEX NAME)

PAGE 1-A







RE.CNT 16 THERE ARE 16 CITED REFERENCES AVAILABLE FOR THIS RECORD  
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L6 ANSWER 3 OF 22 CAPLUS COPYRIGHT 2007 ACS on STN  
AN 2004:830103 CAPLUS  
DN 142:1066  
TI Centrally Acting and Metabolically Stable Thyrotropin-Releasing Hormone  
Analogues by Replacement of Histidine with Substituted Pyridinium  
AU Prokai, Laszlo; Prokai-Tatrai, Katalin; Zharikova, Alevtina D.; Nguyen,  
Vien; Perjesi, Pal; Stevens, Stanley M., Jr.  
CS Department of Medicinal Chemistry, University of Florida, Gainesville, FL,  
32610, USA  
SO Journal of Medicinal Chemistry (2004), 47(24), 6025-6033  
CODEN: JMCMAR; ISSN: 0022-2623  
PB American Chemical Society  
DT Journal  
LA English

OS CASREACT 142:1066

AB Metabolically stable and centrally acting TSH-releasing hormone (TRH) analogs were designed by replacing the central histidine with substituted pyridinium moieties. Their analeptic and acetylcholine-releasing actions were evaluated to assess their potency as central nervous system (CNS) agents. A strong exptl. connection between these two CNS-mediated actions of the TRH analogs was obtained in subject animals. The analog 3-(aminocarbonyl)-1-(3-[2-(aminocarbonyl)pyrrolidin-1-yl]-3-oxo-2-[[5-oxopyrrolidin-2-yl)carbonyl]amino}propyl)pyridinium (1a) showed the highest (TRH-equivalent) potency and longest, dose-dependent duration of action from a series of homologous compds. in antagonizing pentobarbital-induced narcosis when administered i.v. in its CNS-permeable prodrug form (2a) obtained via reduction of the pyridinium moiety to the nonionic dihydropyridine. The maximum change in hippocampal acetylcholine concentration upon perfusion of the pyridinium-containing tripeptides into the hippocampus of rats was also achieved with 1a. No binding to the endocrine TRH receptor was measured for the TRH analogs reported here; therefore, our design afforded a novel lead for centrally acting TRH analogs. We have also demonstrated the benefits of the prodrug approach on the pharmacokinetics and brain uptake/retention of pyridinium-containing TRH analogs (measured by in vivo microdialysis sampling) upon systemic administration.

IT 797054-98-9P  
RL: PAC (Pharmacological activity); PRP (Properties); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)  
(preparation of centrally acting and metabolically stable TSH-releasing hormone analogs by replacement of histidine with substituted pyridinium)

RN 797054-98-9 CAPLUS

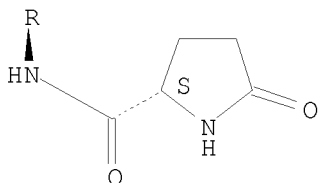
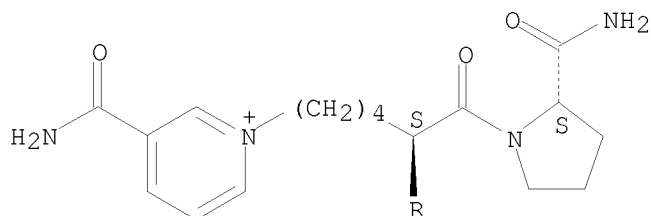
CN L-Prolinamide, 5-oxo-L-prolyl-6-[3-(aminocarbonyl)pyridinio]-L-norleucyl-, salt with trifluoroacetic acid (1:1) (9CI) (CA INDEX NAME)

CM 1

CRN 738575-25-2

CMF C22 H31 N6 O5

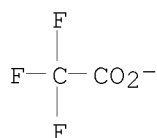
Absolute stereochemistry.



CM 2

CRN 14477-72-6

CMF C2 F3 O2



RE.CNT 47 THERE ARE 47 CITED REFERENCES AVAILABLE FOR THIS RECORD  
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L6 ANSWER 4 OF 22 CAPLUS COPYRIGHT 2007 ACS on STN

AN 2004:610055 CAPLUS

DN 141:157473

TI Preparation of amino acid derivatives as antibacterial agents

IN Anderson, Neils H.; Bowman, Jason; Erwin, Alice; Harwood, Eric; Kline,  
Toni; Mdluli, Khisimuzi; Ng, Simon; Pfister, Keith B.; Shawar, Ribhi;  
Wagman, Allan; Yabannavar, Asha

PA Chiron Corporation, USA

SO PCT Int. Appl., 324 pp.

CODEN: PIXXD2

DT Patent

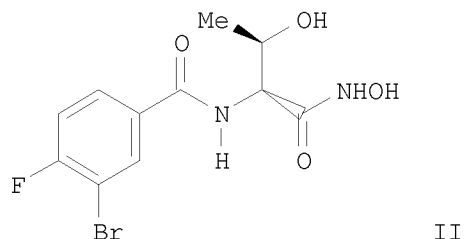
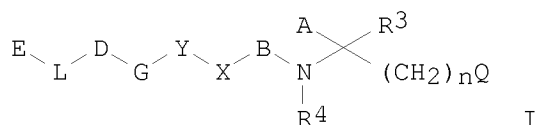
LA English

FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 2004062601	A2	20040729	WO 2004-US433	20040108
	WO 2004062601	A3	20050421		
	W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC,				

LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ

AU	2004204760	A1	20040729	AU	2004-204760	20040108
CA	2512582	A1	20040729	CA	2004-2512582	20040108
US	2004229955	A1	20041118	US	2004-754928	20040108
EP	1618087	A2	20060125	EP	2004-700887	20040108
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, SK						
CN	1777577	A	20060524	CN	2004-80005935	20040108
JP	2006519772	T	20060831	JP	2006-500858	20040108
MX	2005PA07394	A	20050912	MX	2005-PA7394	20050707
IN	2005KN01343	A	20060915	IN	2005-KN1343	20050712
US	2006154988	A1	20060713	US	2005-187708	20050722
US	2007244197	A1	20071018	US	2006-417346	20060503
PRAI	US 2003-438523P	P	20030108			
	US 2003-466974P	P	20030430			
	US 2003-520211P	P	20031113			
	US 2004-754928	A1	20040108			
	WO 2004-US433	W	20040108			
OS	MARPAT 141:157473					
GI						



AB Title compds. I [E = absent or H, (un)substituted-alkyl, -alkenyl, -aryl, etc.; L = absent or CONH, NHCO, (un)substituted alkyl, etc.; D = absent or (un)substituted-cycloalkyl, -aryl, -heterocyclyl or -heteroaryl; G = absent or alkene, alkyne, CO, etc.; Y = (un)substituted-cycloalkyl, -aryl, -heterocyclyl or -heteroaryl; X = CO, alkylcarbonyl, alkenylcarbonyl, alkynylcarbonyl, methylene, or when B is absent X and A together form heterocyclic ring; B = absent or substituted aminoalkylcarbonyl; R3 = H or (un)substituted alkyl, or R3 and A together form a cycloalkyl or heterocyclic ring; R4 = H or (un)substituted alkyl, or R4 and A together form a heterocyclic ring; n = 0-2; A = H, acetylene, alkyl, etc.; Q = absent or substituted amide, SH, SO2NH2, CO2H, etc.] are disclosed: As well as stereoisomers, pharmaceutically acceptable salts, esters, and prodrugs thereof; pharmaceutical compns. comprising such compds.; methods of treating bacterial infections by the administration of such compds.; and processes for the preparation of the compds. Thus, e.g., II was prepared via

amidation of 3-bromo-4-fluorobenzoic acid with L-threonine Me ester hydrochloride followed by substitution with hydroxylamine hydrochloride. This invention pertains generally to treating infections caused by gram-neg. bacteria. More specifically, the invention described pertains to treating gram-neg. infections by inhibiting activity of UDP-3-O-(R-3-hydroxydecanoyl)-N-acetylglucosamine deacetylase (LpxC). Many of I displayed an IC50 value of less than 10  $\mu$ M with respect to inhibition of LpxC.

IT 728872-42-2P

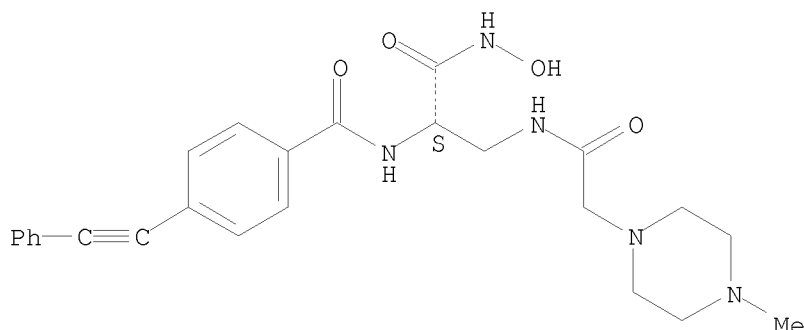
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(drug candidate; preparation of amino acid derivs. as antibacterial agents)

RN 728872-42-2 CAPLUS

CN 1-Piperazineacetamide, N-[(2S)-3-(hydroxyamino)-3-oxo-2-[[4-(phenylethynyl)benzoyl]amino]propyl]-4-methyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L6 ANSWER 5 OF 22 CAPLUS COPYRIGHT 2007 ACS on STN

AN 2004:589539 CAPLUS

DN 141:123573

TI Preparation of (hetero)arylcarboxamides as factor Xa inhibitors

IN Liebeschuetz, John Walter; Sheehan, Scott Martin; Watson, Brian Morgan

PA Eli Lilly and Company, USA

SO PCT Int. Appl., 75 pp.

CODEN: PIXXD2

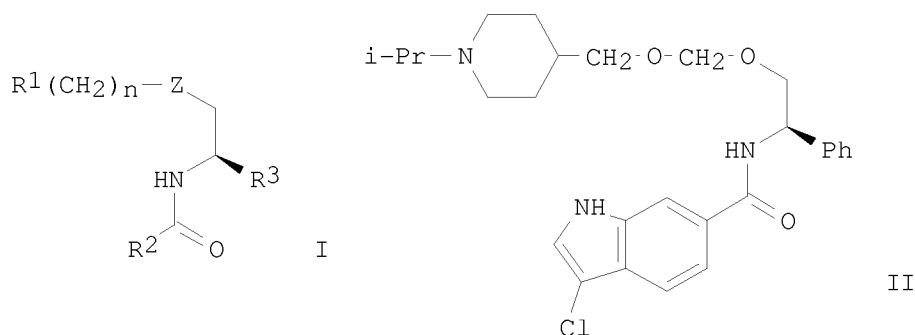
DT Patent

LA English

FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 2004060872	A1	20040722	WO 2003-US39101	20031222
	W:	AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW			
	RW:	BW, GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK,			

TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG  
 AU 2003296393 A1 20040729 AU 2003-296393 20031222  
 EP 1581493 A1 20051005 EP 2003-814680 20031222  
 R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT,  
 IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, SK  
 US 2006052606 A1 20060309 US 2005-539372 20050616  
 PRAI US 2002-436625P P 20021230  
 WO 2003-US39101 W 20031222  
 OS MARPAT 141:123573  
 GI



AB Compds. of formula I [ $R^1$  = pyrrolidinyl, (substituted) piperidinyl, (substituted) piperazinyl;  $R^2$  = (substituted) Ph, indolyl or benzothiophenyl;  $R^3$  = (substituted) Ph, pyridyl, furyl, naphthyl, cycloalkyl, alkyl, etc.;  $Z$  =  $CH_2$ , O, (substituted) NH;  $n$  = 1-3] are prepared as inhibitors of the serine protease Factor Xa and are useful in the treatment of thrombotic disorders. Thus, II was prepared in several steps. The prepared compds. had  $K_{ass}$  values  $> 1 \times 10^6$  L/mol in the enzyme inhibition assay.

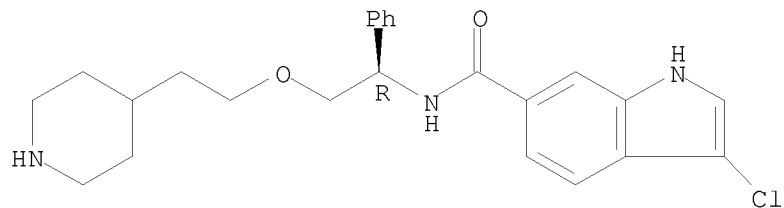
IT 724463-08-5P 724463-09-6P 724463-10-9P  
 RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)  
 (preparation of (hetero)arylcarboxamides as factor Xa inhibitors)

RN 724463-08-5 CAPLUS

CN 1H-Indole-6-carboxamide, 3-chloro-N-[(1R)-1-phenyl-2-[2-(4-piperidinyl)ethoxy]ethyl]-, hydrochloride (9CI) (CA INDEX NAME)

Absolute stereochemistry.

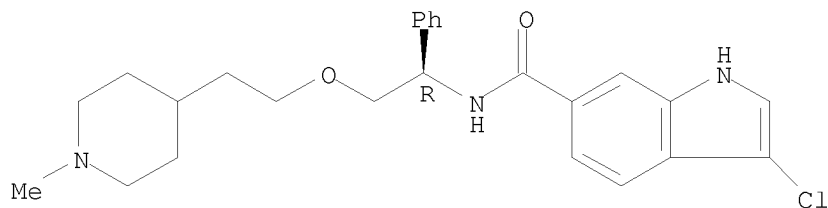
10/539372



●x HCl

RN 724463-09-6 CAPLUS  
CN 1H-Indole-6-carboxamide, 3-chloro-N-[(1R)-2-[2-(1-methyl-4-piperidinyl)ethoxy]-1-phenylethyl]-, hydrochloride (9CI) (CA INDEX NAME)

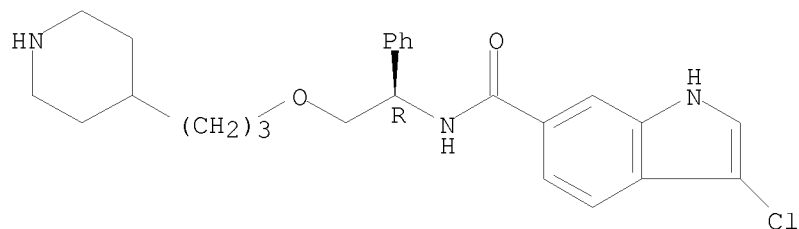
Absolute stereochemistry.



●x HCl

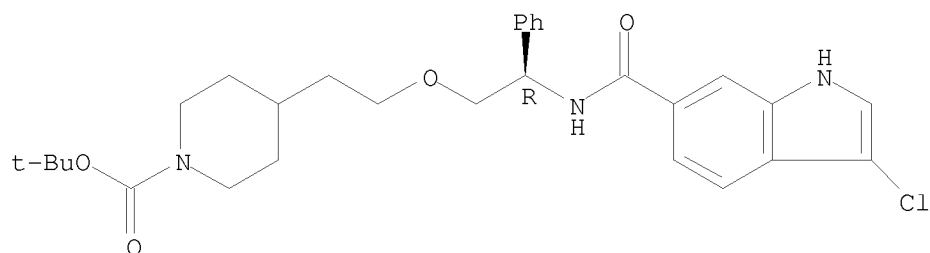
RN 724463-10-9 CAPLUS  
CN 1H-Indole-6-carboxamide, 3-chloro-N-[(1R)-1-phenyl-2-[3-(4-methylpiperidinyl)propoxy]ethyl]- (CA INDEX NAME)

Absolute stereochemistry.



IT 724463-63-2P  
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)  
(preparation of (hetero)arylcarboxamides as factor Xa inhibitors)  
RN 724463-63-2 CAPLUS  
CN 1-Piperidinecarboxylic acid, 4-[2-[(2R)-2-[[[3-chloro-1H-indol-6-yl]carbonyl]amino]-2-phenylethoxy]ethyl]-, 1,1-dimethylethyl ester (CA INDEX NAME)

Absolute stereochemistry.



L6 ANSWER 6 OF 22 CAPLUS COPYRIGHT 2007 ACS on STN

AN 2004:308415 CAPLUS

DN 140:321240

TI Preparation of lactam-containing diaminoalkanes,  $\beta$ -amino acids,  $\alpha$ -amino acids and derivatives thereof as factor Xa inhibitors

IN Qiao, Jennifer X.; Han, Wei

PA Bristol-Myers Squibb Company, USA

SO PCT Int. Appl., 172 pp.

CODEN: PIXXD2

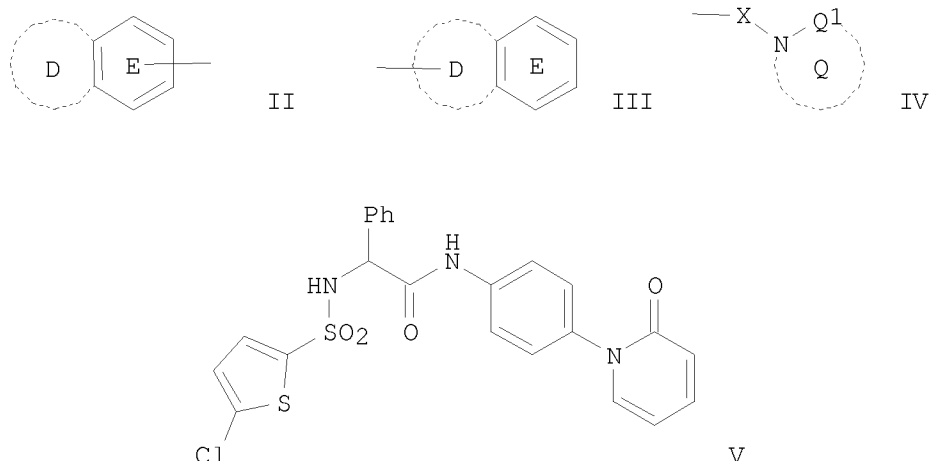
DT Patent

LA English

FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 2004031145	A2	20040415	WO 2003-US31079	20031001
	WO 2004031145	A3	20040701		
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	RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
	US 2004077635	A1	20040422	US 2003-677063	20031001
	AU 2003279735	A1	20040423	AU 2003-279735	20031001
	EP 1558606	A2	20050803	EP 2003-773077	20031001
	R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, SK				
	US 2007129361	A1	20070607	US 2007-622484	20070112
PRAI	US 2002-415366P	P	20021002		
	US 2002-417208P	P	20021009		
	US 2003-677063	A1	20031001		
	WO 2003-US31079	W	20031001		
OS	MARPAT 140:321240				
GI					





AB The title compds. PMM1 [I; one of P and M1 = G and the other -AB; G = II, III (wherein ring D, including the two carbon atoms of ring E to which it is attached, is (un)substituted 5-6 membered ring consisting of carbon atoms and 0-3 heteroatoms selected from N, O, S(O)0-2; ring D may contain 0-3 ring double bonds; ring E = (un)substituted Ph, pyridyl, pyrimidinyl, etc.; alternatively, ring D is absent); M = (un)substituted 3-8 membered linear chain consisting of carbon atoms, carbonyl groups, thiocarbonyl, heteroatoms, and there are 0-2 double bonds and 0-1 triple bond; A = (un)substituted carbocycle, 5-12 membered heterocycle; B = IV (wherein Q1 = CO, SO<sub>2</sub>; ring Q = (un)substituted 4-8 membered monocyclic or bicyclic ring optionally containing optionally heteroatoms, and optionally fused, etc.; X = absent, CO, SO, SO<sub>2</sub>, etc.)], useful as inhibitors of trypsin-like serine proteases, specifically factor Xa for treating thromboembolic disorder, were prepared E.g., a 3-step synthesis of V, starting from 1-(4-aminophenyl)-1H-pyridin-2-one and Boc-DL-PHG-OH, was given. The number of compds. I were found to exhibit K<sub>i</sub>'s of ≤ 10 μM against human factor Xa. The pharmaceutical composition comprising the compound I is claimed.

IT 678175-26-3P 678175-27-4P 678175-33-2P  
678175-64-9P 678175-65-0P 678175-70-7P  
678176-04-0P 678176-05-1P 678176-10-8P  
678176-56-2P 678176-57-3P 678176-62-0P  
678176-96-0P 678177-12-3P 678177-13-4P  
678177-25-8P 678177-41-8P 678177-42-9P

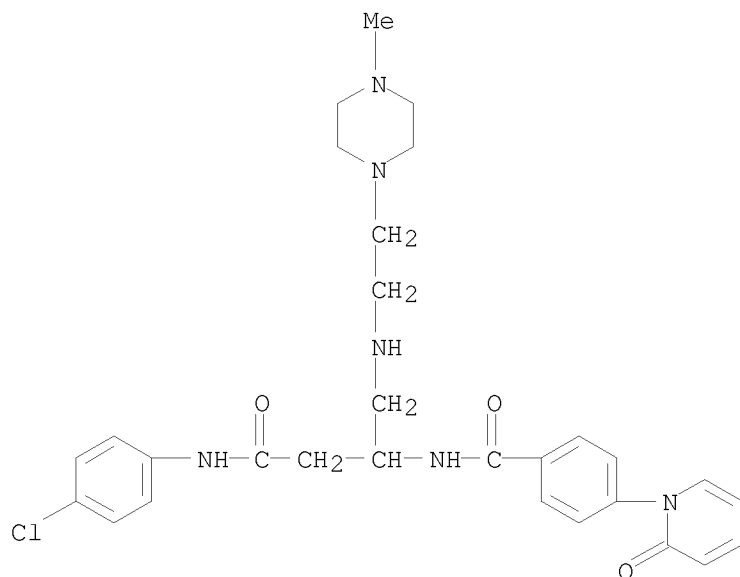
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(preparation of lactam-containing diaminoalkanes, β-amino acids, α-amino acids and derivs. thereof as factor Xa inhibitors for treating thromboembolic disorder)

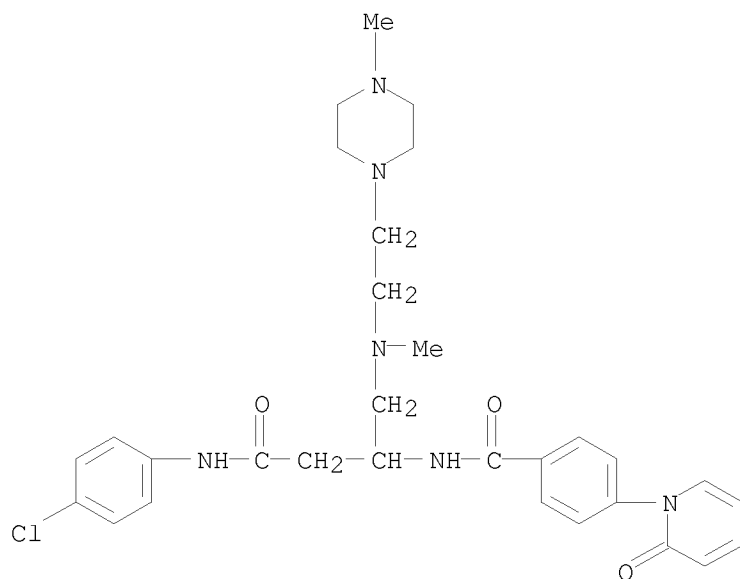
RN 678175-26-3 CAPLUS

CN Benzamide, N-[3-[(4-chlorophenyl)amino]-1-[[[2-(4-methyl-1-piperazinyl)ethyl]amino]methyl]-3-oxopropyl]-4-(2-oxo-1(2H)-pyridinyl)-(CA INDEX NAME)

10/539372

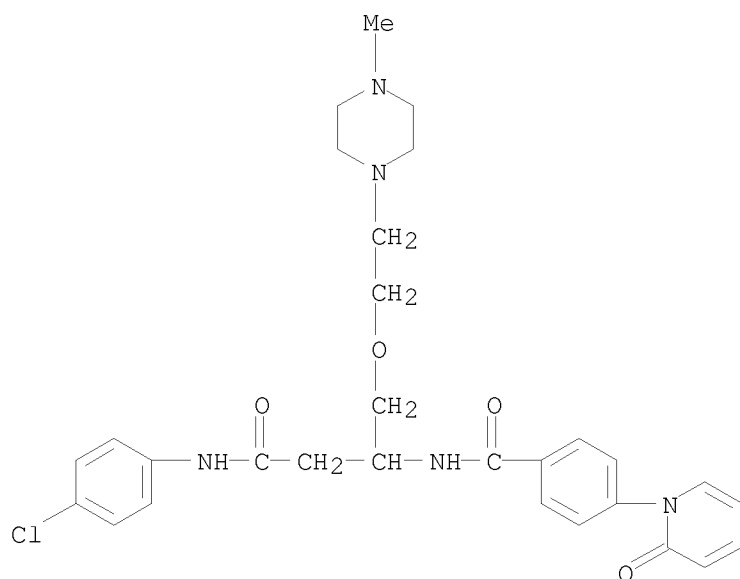


RN 678175-27-4 CAPLUS  
CN Benzamide, N-[3-[(4-chlorophenyl)amino]-1-[[methyl[2-(4-methyl-1-piperazinyl)ethyl]amino]methyl]-3-oxopropyl]-4-(2-oxo-1(2H)-pyridinyl)-  
(CA INDEX NAME)

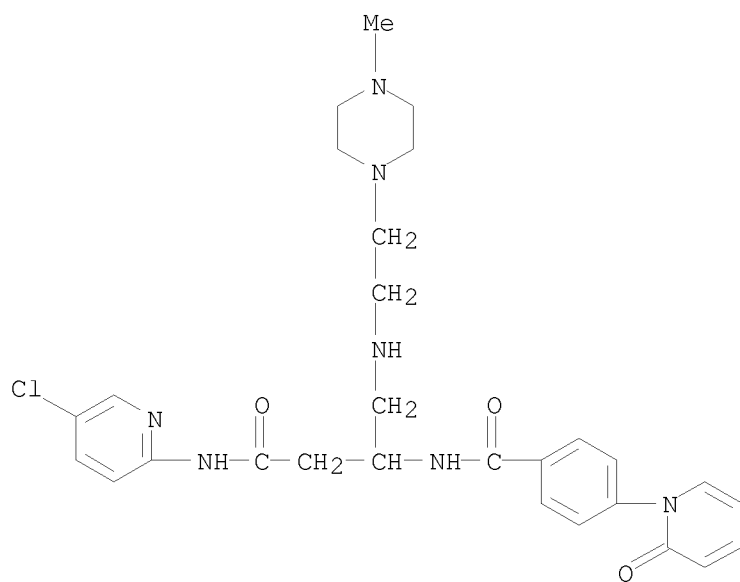


RN 678175-33-2 CAPLUS  
CN Benzamide, N-[3-[(4-chlorophenyl)amino]-1-[[2-(4-methyl-1-piperazinyl)ethoxy]methyl]-3-oxopropyl]-4-(2-oxo-1(2H)-pyridinyl)- (CA  
INDEX NAME)

10/539372

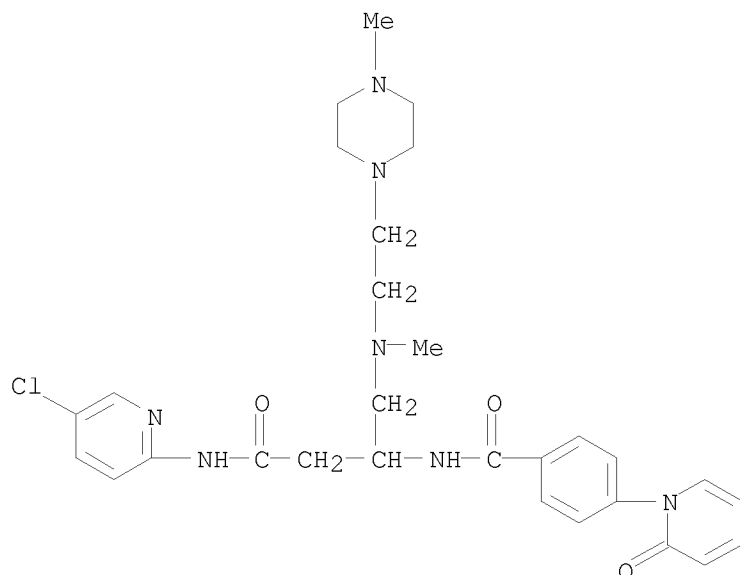


RN 678175-64-9 CAPLUS  
CN Benzamide, N-[3-[(5-chloro-2-pyridinyl)amino]-1-[[2-(4-methyl-1-piperazinyl)ethyl]amino]methyl]-3-oxopropyl]-4-(2-oxo-1(2H)-pyridinyl)-  
(CA INDEX NAME)

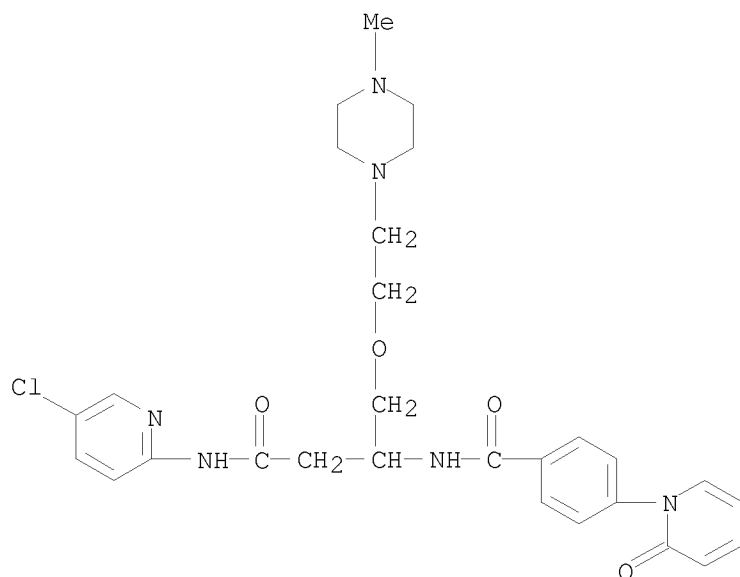


RN 678175-65-0 CAPLUS  
CN Benzamide, N-[3-[(5-chloro-2-pyridinyl)amino]-1-[[methyl[2-(4-methyl-1-piperazinyl)ethyl]amino]methyl]-3-oxopropyl]-4-(2-oxo-1(2H)-pyridinyl)-  
(CA INDEX NAME)

10/539372

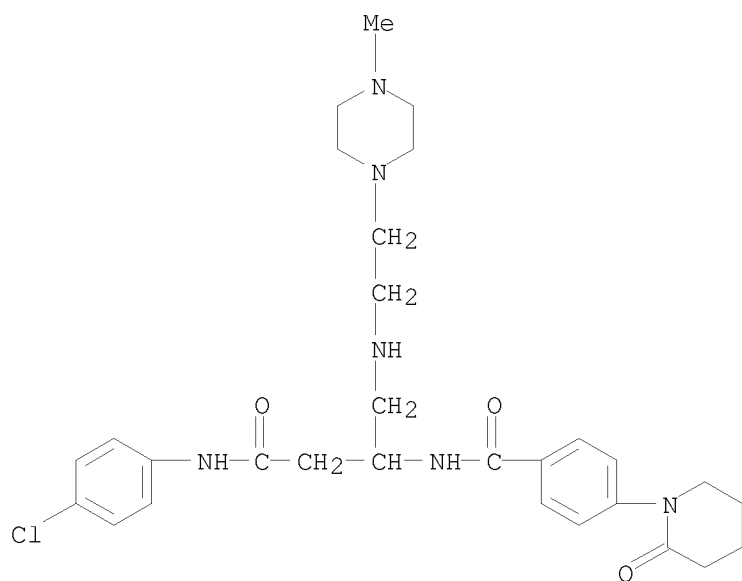


RN 678175-70-7 CAPLUS  
CN Benzamide, N-[3-[(5-chloro-2-pyridinyl)amino]-1-[[2-(4-methyl-1-piperazinyl)ethoxy]methyl]-3-oxopropyl]-4-(2-oxo-1(2H)-pyridinyl)- (CA INDEX NAME)

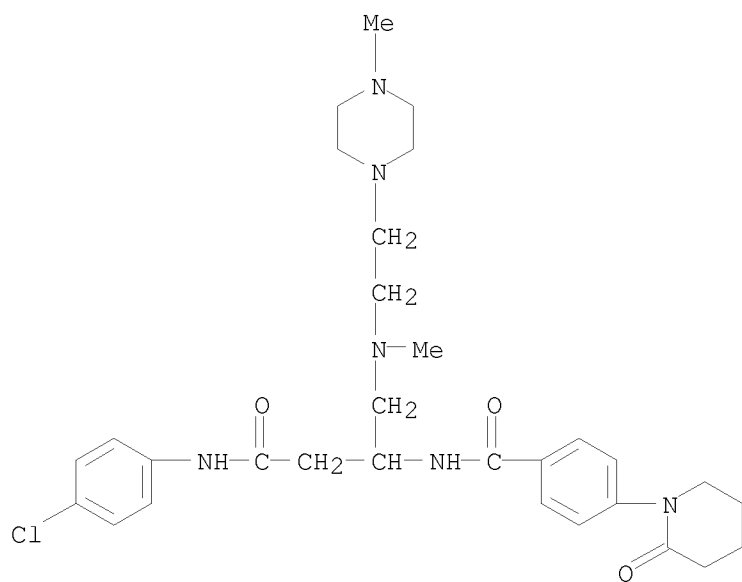


RN 678176-04-0 CAPLUS  
CN Benzamide, N-[3-[(4-chlorophenyl)amino]-1-[[2-(4-methyl-1-piperazinyl)ethyl]amino]methyl]-3-oxopropyl]-4-(2-oxo-1-piperidinyl)- (CA INDEX NAME)

10/539372

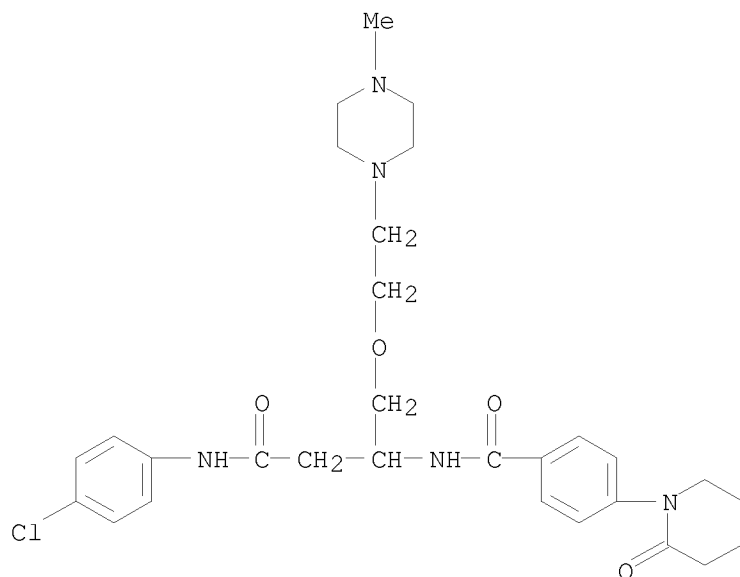


RN 678176-05-1 CAPLUS  
 CN Benzamide, N-[3-[(4-chlorophenyl)amino]-1-[[methyl[2-(4-methyl-1-piperazinyl)ethyl]amino]methyl]-3-oxopropyl]-4-(2-oxo-1-piperidinyl)- (CA INDEX NAME)

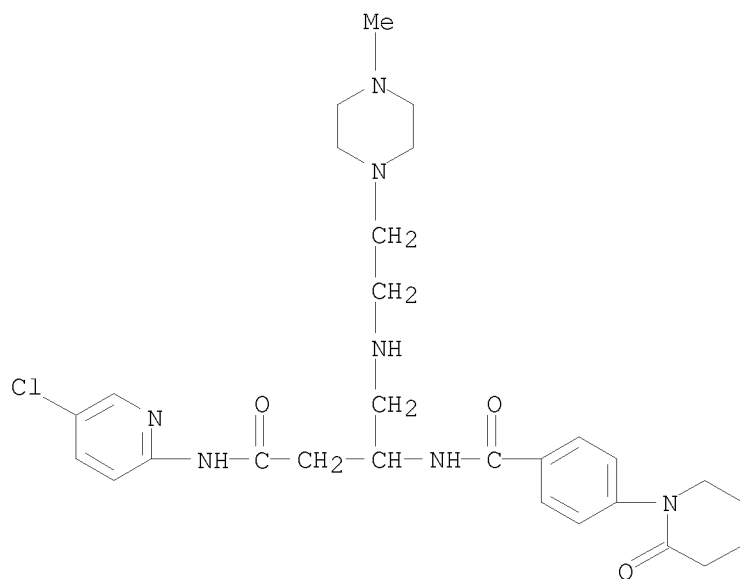


RN 678176-10-8 CAPLUS  
 CN Benzamide, N-[3-[(4-chlorophenyl)amino]-1-[[2-(4-methyl-1-piperazinyl)ethoxy]methyl]-3-oxopropyl]-4-(2-oxo-1-piperidinyl)- (CA INDEX NAME)

10/539372

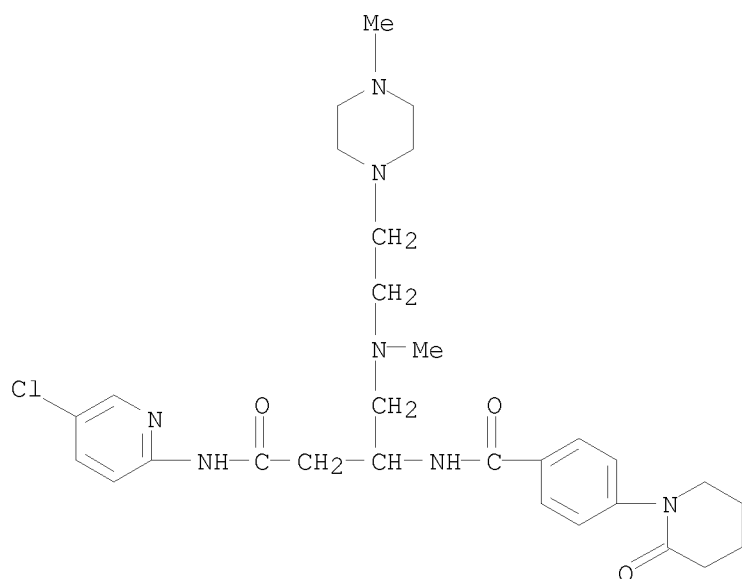


RN 678176-56-2 CAPLUS  
 CN Benzamide, N-[3-[(5-chloro-2-pyridinyl)amino]-1-[[[2-(4-methyl-1-piperazinyl)ethyl]amino]methyl]-3-oxopropyl]-4-(2-oxo-1-piperidinyl)- (CA INDEX NAME)

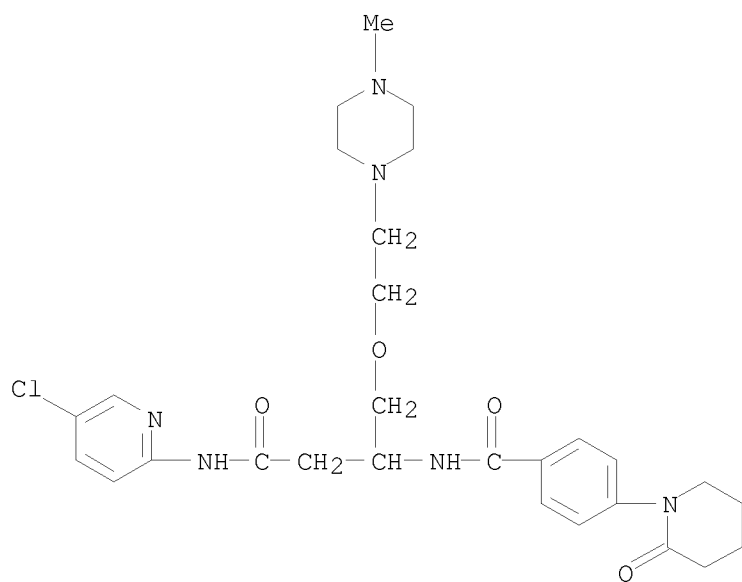


RN 678176-57-3 CAPLUS  
 CN Benzamide, N-[3-[(5-chloro-2-pyridinyl)amino]-1-[[methyl[2-(4-methyl-1-piperazinyl)ethyl]amino]methyl]-3-oxopropyl]-4-(2-oxo-1-piperidinyl)- (CA INDEX NAME)

10/539372

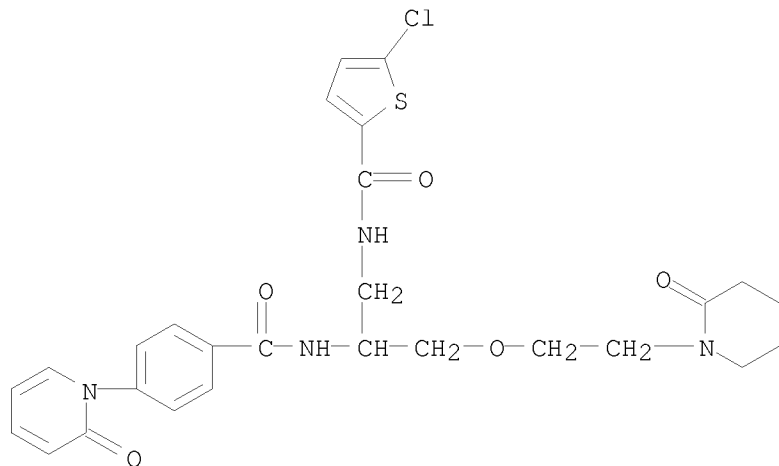


RN 678176-62-0 CAPLUS  
CN Benzamide, N-[3-[(5-chloro-2-pyridinyl)amino]-1-[[2-(4-methyl-1-piperazinyl)ethoxy]methyl]-3-oxopropyl]-4-(2-oxo-1-piperidinyl)- (CA INDEX NAME)



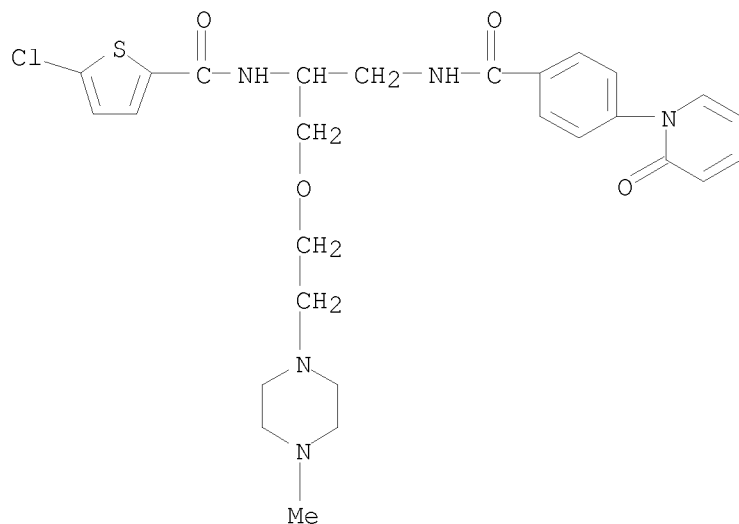
RN 678176-96-0 CAPLUS  
CN 2-Thiophenecarboxamide, 5-chloro-N-[3-[2-(2-oxo-1-piperidinyl)ethoxy]-2-[[4-(2-oxo-1(2H)-pyridinyl)benzoyl]amino]propyl]- (CA INDEX NAME)

10/539372



RN 678177-12-3 CAPLUS

CN 2-Thiophenecarboxamide, 5-chloro-N-[1-[[2-(4-methyl-1-piperazinyl)ethoxy]methyl]-2-[[4-(2-oxo-1(2H)-pyridinyl)benzoyl]amino]ethyl]-2-methyl-1-piperazinecarboxamide (CA INDEX NAME)

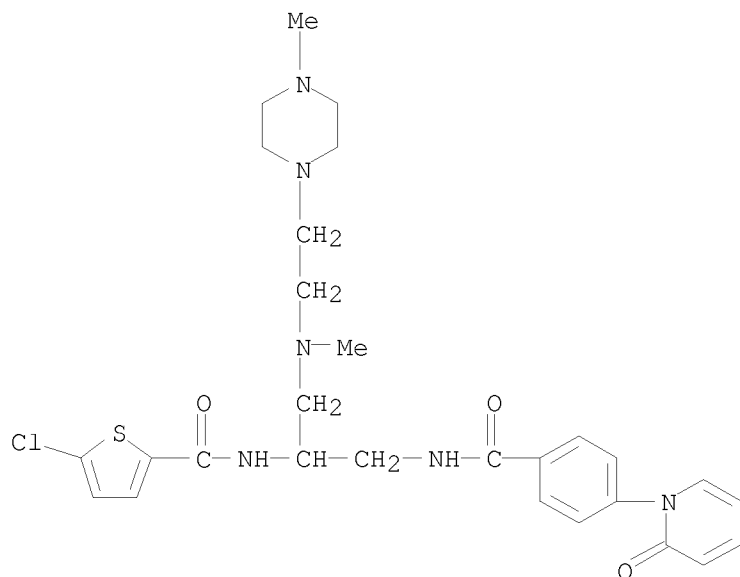


RN 678177-13-4 CAPLUS

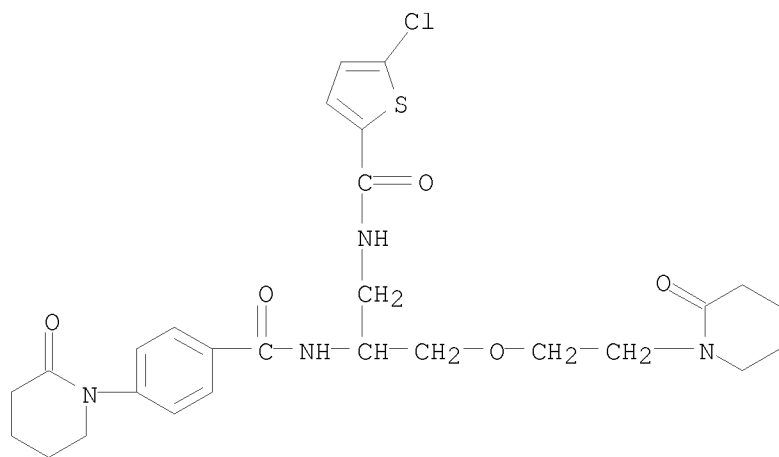
CN 2-Thiophenecarboxamide, 5-chloro-N-[1-[[methyl[2-(4-methyl-1-piperazinyl)ethyl]amino]methyl]-2-[[4-(2-oxo-1(2H)-pyridinyl)benzoyl]amino]ethyl]-2-methyl-1-piperazinecarboxamide (CA INDEX NAME)



10/539372

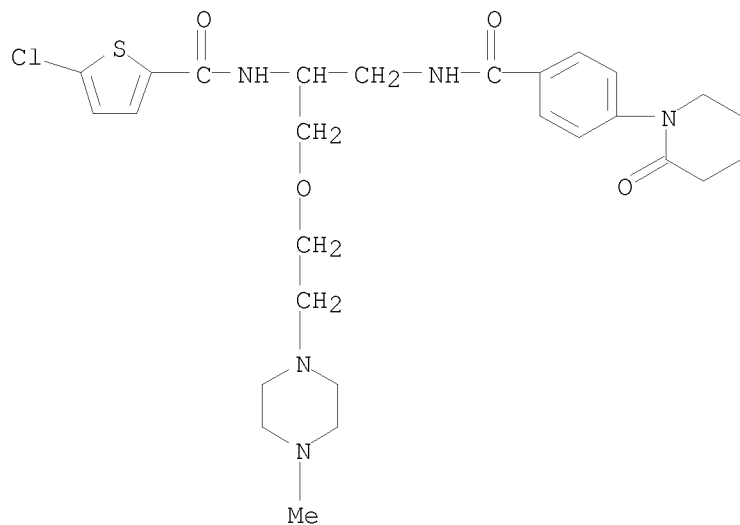


RN 678177-25-8 CAPLUS  
 CN 2-Thiophenecarboxamide, 5-chloro-N-[2-[[4-(2-oxo-1-piperidinyloxy)benzoyl]amino]-3-[2-(2-oxo-1-piperidinyloxy)ethoxy]propyl]- (CA INDEX NAME)



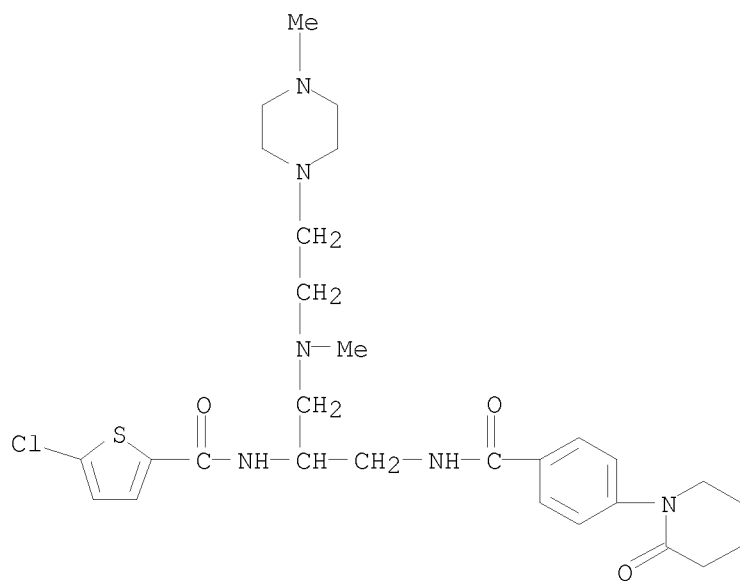
RN 678177-41-8 CAPLUS  
 CN 2-Thiophenecarboxamide, 5-chloro-N-[1-[[2-(4-methyl-1-piperazinyl)ethoxy]methyl]-2-[[4-(2-oxo-1-piperidinyloxy)benzoyl]amino]ethyl]- (CA INDEX NAME)

10/539372



RN 678177-42-9 CAPLUS

CN 2-Thiophenecarboxamide, 5-chloro-N-[1-[[methyl[2-(4-methyl-1-piperazinyl)ethyl]amino]methyl]-2-[[4-(2-oxo-1-piperidinyl)benzoyl]amino]ethyl]- (CA INDEX NAME)



L6 ANSWER 7 OF 22 CAPLUS COPYRIGHT 2007 ACS on STN

AN 2004:182658 CAPLUS

DN 140:235738

TI Preparation of pyrazolopyrimidines as calcium receptor modulators

IN Yasuma, Tsuneo; Mori, Akira; Kawase, Masahiro; Kimura, Hiroyuki; Yoshida, Masato; Gyorkos, Albert Charles; Pratt, Scott Alan; Corrette, Christopher Peter

PA Takeda Chemical Industries, Ltd., Japan; Takeda Pharmaceutical Company Limited

SO PCT Int. Appl., 460 pp.

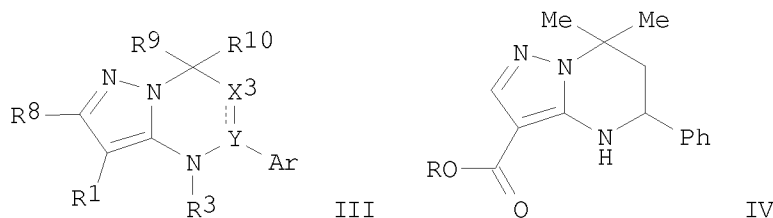
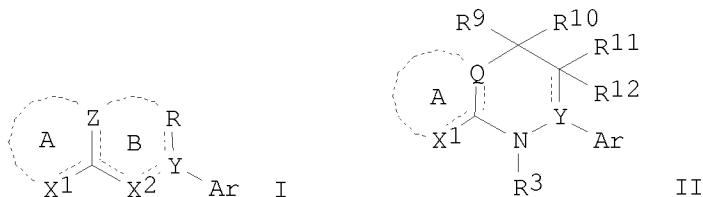
CODEN: PIXXD2

DT Patent

LA English

FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
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	WO 2004017908	A3	20060105		
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	RW:	GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG			
	CA 2494700	A1	20040304	CA 2003-2494700	20030821
	AU 2003265585	A1	20040311	AU 2003-265585	20030821
	EP 1572113	A2	20050914	EP 2003-793273	20030821
	R:	AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, SK			
	JP 2006510582	T	20060330	JP 2004-529835	20030821
	CN 1771231	A	20060510	CN 2003-823938	20030821
	BR 2003013880	A	20071106	BR 2003-13880	20030821
	US 2006079536	A1	20060413	US 2005-525158	20050222
	IN 2005KN00280	A	20060818	IN 2005-KN280	20050225
	NO 2005001328	A	20050315	NO 2005-1328	20050315
PRAI	US 2002-406012P	P	20020826		
	US 2003-466129P	P	20030428		
	WO 2003-US26317	W	20030821		
OS	MARPAT 140:235738				
GI					



AB The title compds. [I; ring A = (un)substituted 5-7 membered ring; ring B = (un)substituted 5-7 membered heterocyclic ring; X1 = (un)substituted CH, CH2, N or NH; X2 = N or (un)substituted NH; Y = C, (un)substituted CH or N; Z = (un)substituted CH, CH2, N or NH; Ar = (un)substituted cyclic group; R = H, (un)substituted alkyl, etc.; and their salts], useful as calcium receptor modulators, were provided. The compds. II, III [wherein ring A = (un)substituted 5-7 membered ring; Q = C, CR5 (R5 = H, alkyl, hydroxyalkyl, etc.), or N; X1 = CR1 (R1 = H, alkyl, hydroxyalkyl, etc.), CR1R2 (R1 as above; R2 = H, heterocyclyl, etc.); R3 = H, alkyl, hydroxyalkyl, aminoalkyl, etc.; Y = C, CR4 (R4 = H, alkyl, hydroxyalkyl, etc.), or N; R8-R12 = H, (un)substituted alkyl, etc.; X3 = a bond, O, (un)oxidized S, N, (un)substituted NH, C1-2 alkylene; or their salts], were also provided. Thus, reacting amidation of the acid IV [R = H] with 4-(F3C)C6H4C(Et)2NH2 afforded 31% IV [R = 4-(F3C)C6H4C(Et)2NH]. Biol. data were given for selected compds. The pharmaceutical composition comprising the compound I is claimed.

IT 667922-27-2P

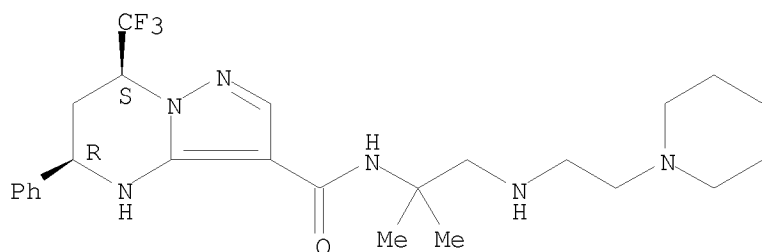
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(preparation of pyrazolopyrimidines as calcium receptor modulators)

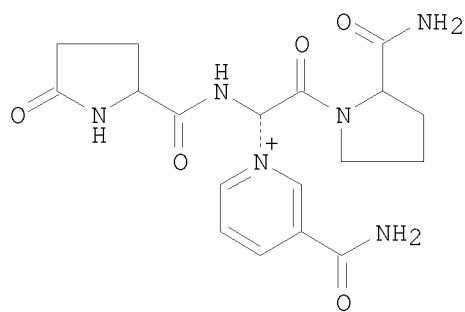
RN 667922-27-2 CAPLUS

CN Pyrazolo[1,5-a]pyrimidine-3-carboxamide, N-[1,1-dimethyl-2-[[2-(1-piperidinyl)ethyl]amino]ethyl]-4,5,6,7-tetrahydro-5-phenyl-7-(trifluoromethyl)-, (5R,7S)-rel- (CA INDEX NAME)

Relative stereochemistry.



L6 ANSWER 8 OF 22 CAPLUS COPYRIGHT 2007 ACS on STN  
 AN 2002:543696 CAPLUS  
 DN 137:353286  
 TI Design, synthesis, and biological evaluation of novel, centrally-acting  
 thyrotropin-releasing hormone analogs  
 AU Prokai-Tatrai, Katalin; Perjesi, Pal; Zharikova, Alevtina D.; Li, Xiaoxu;  
 Prokai, Laszlo  
 CS College of Pharmacy, Center for Drug Discovery, University of Florida,  
 Gainesville, FL, 32610-0497, USA  
 SO Bioorganic & Medicinal Chemistry Letters (2002), 12(16), 2171-2174  
 CODEN: BMCLE8; ISSN: 0960-894X  
 PB Elsevier Science Ltd.  
 DT Journal  
 LA English  
 OS CASREACT 137:353286  
 GI



I

AB Novel, metabolically stable and centrally acting TRH analogs with  
 substituted pyridinium moieties replacing the [His2] residue of the  
 endogenous peptide were prepared by solid-phase Zincke reaction. The  
 1,4-dihydropyridine prodrugs of these analogs obtained after reducing the  
 pyridinium moiety were able to reach the brain and maintain a sustained  
 concentration of the charged, degradation-resistant analogs formed after  
 enzymic  
 oxidation of the prodrug, as manifested by the analeptic action measured in  
 mice. Among the four analogs reported, compound I showed the highest  
 potency and longest duration of action in reducing the  
 pentobarbital-induced sleeping time compared to the parent TRH. No  
 binding to the endocrine TRH-receptor was measured for I; thus, this

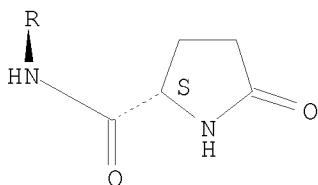
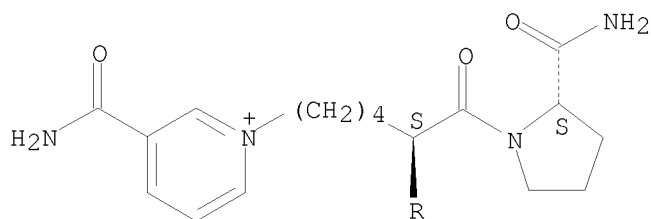
compound emerged as a potent, centrally acting TRH analog.

IT 474520-12-2P  
 RL: ANT (Analyte); PAC (Pharmacological activity); RCT (Reactant); SPN (Synthetic preparation); ANST (Analytical study); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent)  
 (solid-phase synthesis, analeptic action, and receptor binding of TSH-releasing hormone pyridine and dihydropyridine analogs)

RN 474520-12-2 CAPLUS

CN L-Prolinamide, 5-oxo-L-prolyl-6-[3-(aminocarbonyl)pyridinio]-L-norleucyl-, chloride (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RE.CNT 20 THERE ARE 20 CITED REFERENCES AVAILABLE FOR THIS RECORD  
 ALL CITATIONS AVAILABLE IN THE RE FORMAT

L6 ANSWER 9 OF 22 CAPLUS COPYRIGHT 2007 ACS on STN  
 AN 2002:247283 CAPLUS  
 DN 137:6366  
 TI A Solid-Phase Synthetic Route to Unnatural Amino Acids with Diverse Side-Chain Substitutions  
 AU Scott, William L.; O'Donnell, Martin J.; Delgado, Francisca; Alsina, Jordi  
 CS Lilly Research Laboratories, Eli Lilly and Company, Indianapolis, IN, 46285, USA  
 SO Journal of Organic Chemistry (2002), 67(9), 2960-2969  
 CODEN: JOCEAH; ISSN: 0022-3263  
 PB American Chemical Society  
 DT Journal  
 LA English  
 OS CASREACT 137:6366  
 AB Reacting imine derivs. of resin-bound amino acids (i.e., 3,4-dichlorobenzaldehyde Schiff bases of Wang resin-bound Ala or Phe) with  $\alpha,\omega$ -dihaloalkanes provides highly versatile intermediates to racemic  $\alpha,\alpha$ -disubstituted amino acids with a wide variety of

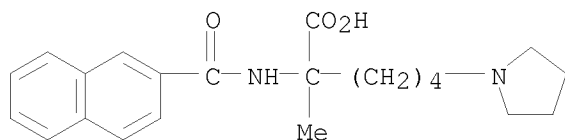
side-chain functionality. Two strategies were developed to convert the intermediate  $\omega$ -chloro or  $\omega$ -bromo derivs. to the desired products. Together, they allow the creation of amino acids with diverse functionalities ( $\omega$ -chlorides, nitriles, azides, acetates, thioacetates, thioethers, secondary and tertiary aliphatic amines, and anilines) placed at varying chain lengths (2-5) from the  $\alpha$ -center of the amino acid.

IT 433220-56-5P

RL: SPN (Synthetic preparation); PREP (Preparation)  
(preparation of side-chain substituted amino acids by alkylating Schiff bases of Phe- or Ala-Wang resins with dihaloalkanes followed by nucleophilic substitutions)

RN 433220-56-5 CAPLUS

CN 1-Pyrrolidinehexanoic acid,  $\alpha$ -methyl- $\alpha$ -[(2-naphthalenylcarbonyl)amino]- (CA INDEX NAME)



RE.CNT 51 THERE ARE 51 CITED REFERENCES AVAILABLE FOR THIS RECORD  
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L6 ANSWER 10 OF 22 CAPLUS COPYRIGHT 2007 ACS on STN

AN 2002:142742 CAPLUS

DN 136:200481

TI Preparation of water-soluble thiazolyl peptide derivatives

IN Naidu, B. Narasimhulu; Li, Wenying; Lam, Kin S.; Sorenson, Margaret E.; Wichtowski, John A.; Connolly, Timothy P.; Ueda, Yasutsugu; Bronson, Joanne J.; Zhang, Yunhui; Kim, Oak K.

PA Bristol-Myers Squibb Company, USA

SO PCT Int. Appl., 90 pp.

CODEN: PIXXD2

DT Patent

LA English

FAN.CNT 1

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2002014354	A1	20020221	WO 2001-US25560	20010815
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
US 2002065219	A1	20020530	US 2001-928468	20010813
AU 2001086497	A5	20020225	AU 2001-86497	20010815
PRAI US 2000-225598P	P	20000815		
WO 2001-US25560	W	20010815		
OS MARPAT 136:200481				

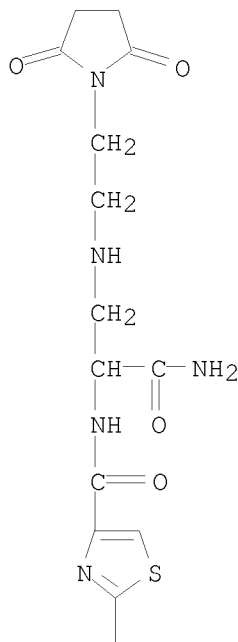
AB Novel thiazolyl peptides R1-Y-CH<sub>2</sub>CH(Q)CONH<sub>2</sub> [Q is a residue of a thiazolyl peptide antibiotic, e.g., nocathiacin I or nosiheptide; Y = S, SO, SO<sub>2</sub> or NR, where R = H, OH, alkoxy, alkanoyl, alkylcarbamoyl, etc.; R1 = 1-azabicyclo[2.2.2]oct-3-yl or N-oxide, [(CH<sub>2</sub>)<sub>20</sub>]1-3(CH<sub>2</sub>)<sub>2</sub>R4' (R4' = OH, amino, phenylmethyl), or (un)substituted alkyl] were prepared for use in pharmaceutical compns. for the treatment of serious bacterial infections. Thus, a peptide prepared by Michael addition reaction of nocathiacin I with 1-methylpiperazine showed in vitro antibiotic activity 0.25, 0.125, and 0.5 µg/mL (MIC) against Staphylococcus aureus, Streptococcus pneumoniae, and Enterococcus faecalis, resp.

IT 401826-04-8P 401826-37-7P 401826-74-2P  
 RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)  
 (preparation of water-soluble thiazolyl peptide derivs.)

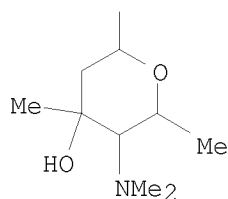
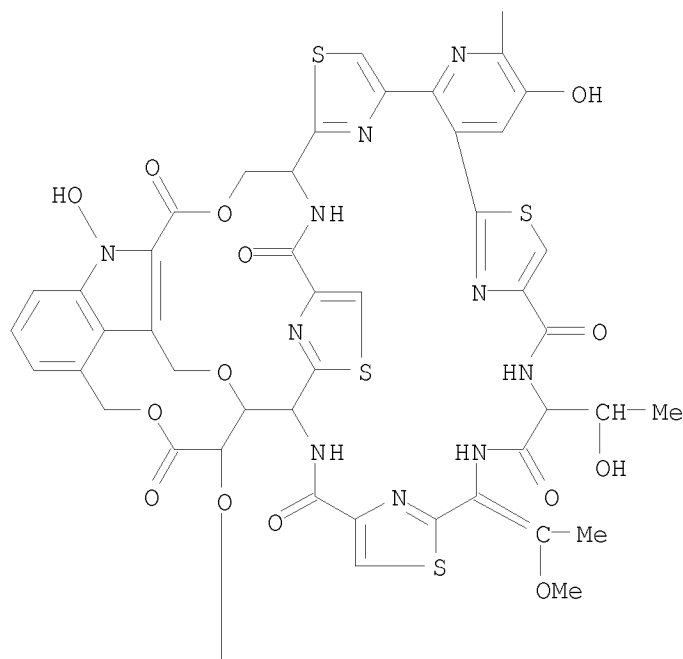
RN 401826-04-8 CAPLUS

CN 4-Thiazolecarboxamide, N-[2-amino-1-[[[2-(2,5-dioxo-1-pyrrolidinyl)ethyl]amino]methyl]-2-oxoethyl]-2-[(11S,14E,21S,22R,33S,49S)-9,10,11,12,13,14,19,20,21,22,29,30,32,33-tetradecahydro-3,29-dihydroxy-11-[(1R)-1-hydroxyethyl]-14-(1-methoxyethylidene)-9,12,19,30,40,48-hexaoxo-49-[[2,4,6-trideoxy-4-(dimethylamino)-3-C-methyl-α-L-lyxo-hexopyranosyl]oxy]-22,25-(ethanoxymethano)-8,5:18,15:37,34-trinitrilo-21,33-([2,4]-endo-thiazolomethanimino)-5H,15H,24H,34H-pyrido[3',2':20,21][1,28,8,18,24,4,11,14]dioxatrithiatriazacyclodotriacontino[30,31-b]indol-2-yl]- (9CI) (CA INDEX NAME)

PAGE 1-A



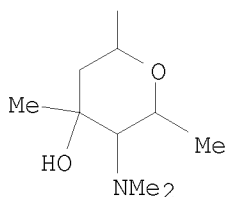




RN	401826-37-7	CAPLUS
CN	4-Thiazolecarboxamide, N-[2-amino-1-[[methyl[2-(1-piperidinyl)ethyl]amino]methyl]-2-oxoethyl]-2-[(11S,14E,21S,22R,33S,49S)-9,10,11,12,13,14,19,20,21,22,29,30,32,33-tetradecahydro-3,29-dihydroxy-11-[(1R)-1-hydroxyethyl]-14-(1-methoxyethylidene)-9,12,19,30,40,48-hexaoxo-49-[[2,4,6-trideoxy-4-(dimethylamino)-3-C-methyl- $\alpha$ -L-lyxo-hexopyranosyl]oxy]-22,25-(ethanoxymethano)-8,5:18,15:37,34-trinitrilo-21,33-([2,4]-endo-thiazolomethanimino)-5H,15H,24H,34H-pyrido[3',2':20,21][1,28,8,18,24,4,11,14]dioxatrithiatriazacyclodotriacontino[30,31-b]indol-2-yl]- (9CI) (CA INDEX NAME)	

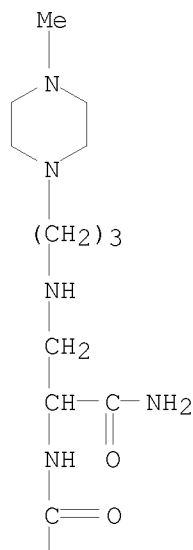


PAGE 3-A

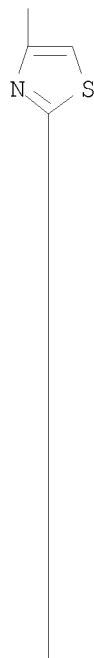


RN 401826-74-2 CAPLUS  
 CN 4-Thiazolecarboxamide, N-[2-amino-1-[[[3-(4-methyl-1-piperazinyl)propyl]amino]methyl]-2-oxoethyl]-2-[(11S,14E,21S,22R,33S,49S)-9,10,11,12,13,14,19,20,21,22,29,30,32,33-tetradecahydro-3,29-dihydroxy-11-[(1R)-1-hydroxyethyl]-14-(1-methoxyethylidene)-9,12,19,30,40,48-hexaoxo-49-[[2,4,6-trideoxy-4-(dimethylamino)-3-C-methyl- $\alpha$ -L-lyxo-hexopyranosyl]oxy]-22,25-(ethanoxymethano)-8,5:18,15:37,34-trinitrilo-21,33-([2,4]-endo-thiazolomethanimino)-5H,15H,24H,34H-pyrido[3',2':20,21][1,28,8,18,24,4,11,14]dioxatrithiatriazacyclodotriacontino[30,31-b]indol-2-yl]- (9CI) (CA INDEX NAME)

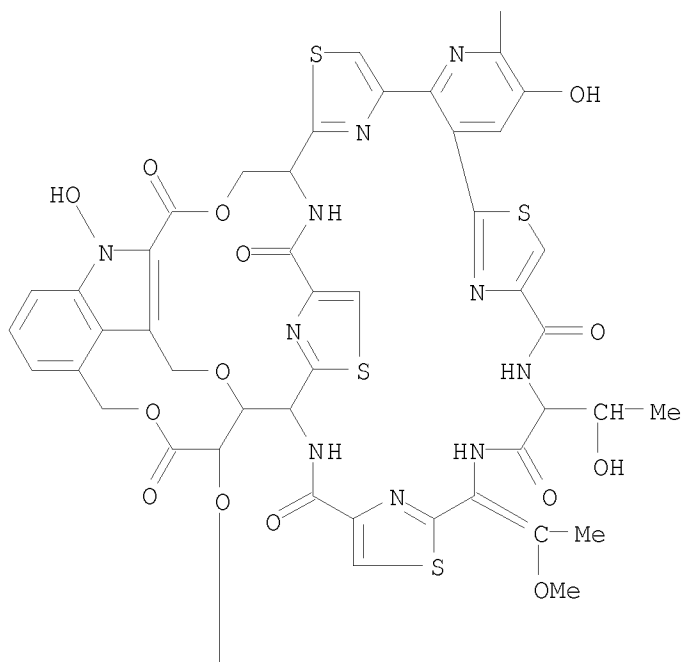
PAGE 1-A

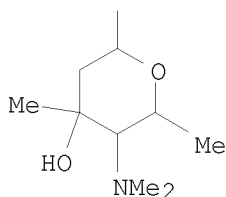


PAGE 2-A



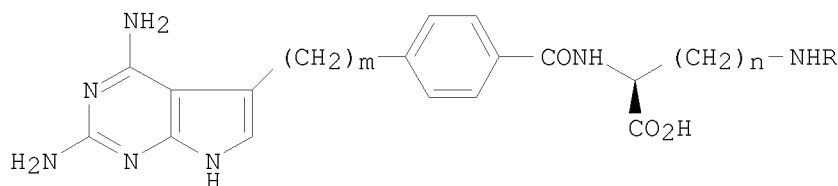
PAGE 3-A





RE.CNT 2 THERE ARE 2 CITED REFERENCES AVAILABLE FOR THIS RECORD  
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L6 ANSWER 11 OF 22 CAPLUS COPYRIGHT 2007 ACS on STN  
AN 2000:643793 CAPLUS  
DN 133:329128  
TI Non-glutamate type pyrrolo[2,3-d]pyrimidine antifolates. III. Synthesis and biological properties of N $\omega$ -masked ornithine analogs  
AU Itoh, Fumio; Yoshioka, Yoshio; Yukishige, Koichi; Yoshida, Sei; Ootsu, Koichiro; Akimoto, Hiroshi  
CS Medicinal Chemistry Research Laboratories, Takeda Chemical Industries, Ltd., Osaka, 532-8686, Japan  
SO Chemical & Pharmaceutical Bulletin (2000), 48(9), 1270-1280  
CODEN: CPBTAL; ISSN: 0009-2363  
PB Pharmaceutical Society of Japan  
DT Journal  
LA English  
OS CASREACT 133:329128  
GI



I

AB Non-glutamate type pyrrolo[2,3-d]pyrimidine antifolates I [ $m = 2, 3$ ;  $n = 1-4$ ;  $R = H, CO_2Bu-t, CO_2CH_2Ph, CO(CH_2)_2CO_2H, COCH:CHCO_2H, COC_6H_4CO_2H-2, COC_6H_4CO_2H-4, 2-(1-pyrrolidinylcarbonyl)benzoyl, COC_6H_4OH-2, COC_6H_4(NHAc)-4, SO_2C_6H_4Me-4, SO_2C_6H_4CO_2H-2, CONHC_6H_4F-4, CONHC_6H_4CO_2H-3, CONHC_6H_4-3-B(OH)_3, C_6H_4CO_2H-3, 3-carboxy-2-naphthoyl, etc.] were synthesized and their inhibitory effects on dihydrofolate reductase (DHFR), the growth of murine fibrosarcoma Meth A cells, and methotrexate-resistant human CCRF-CEM cells were examined. A free ornithine analog I ( $m = n = 3, R = H$ ) did not strongly inhibit Meth A cell growth, whereas all N $\omega$ -substituted ornithine analogs ( $R = acyl, sulfonyl, carbamoyl, aryl$ ) exhibited much more potent inhibitory activities against both DHFR and Meth A cell growth. In particular, compds. I [ $m = 2, n = 3,$$

R = COC<sub>6</sub>H<sub>4</sub>CO<sub>2</sub>H-2; m = 2, n = 3, R = 3-carboxy-2-naphthoyl; m = 2, n = 3, R = C<sub>6</sub>H<sub>4</sub>CO<sub>2</sub>H-3] also showed remarkable growth-inhibitory activities against methotrexate-resistant CCRF-CEM cells. These results demonstrate that the potent inhibitory activities of N $\alpha$ -masked ornithine analogs against the growth of Meth A cells and methotrexate-resistant CCRF-CEM cells, results from effective uptake via reduced folate carrier and their potent DHFR inhibition.

IT 149009-83-6P 303957-87-1P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

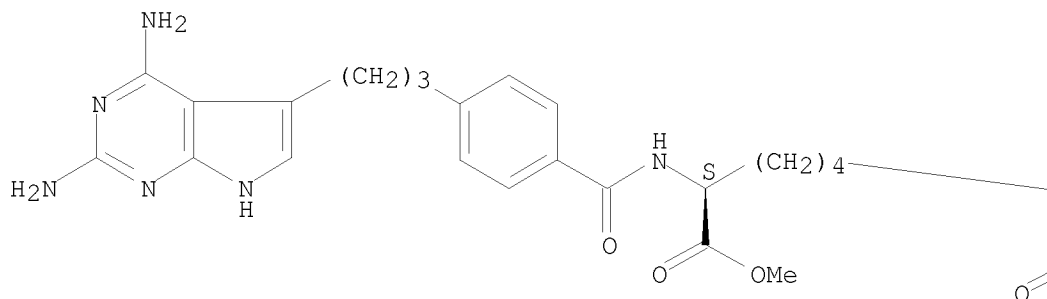
(preparation and antitumor activity of non-glutamate, ornithine-containing pyrrolo[2,3-d]pyrimidine antifolates)

RN 149009-83-6 CAPLUS

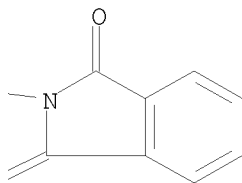
CN 2H-Isoindole-2-hexanoic acid,  $\alpha$ -[[4-[3-(2,4-diamino-1H-pyrrolo[2,3-d]pyrimidin-5-yl)propyl]benzoyl]amino]-1,3-dihydro-1,3-dioxo-, methyl ester, ( $\alpha$ S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A



PAGE 1-B

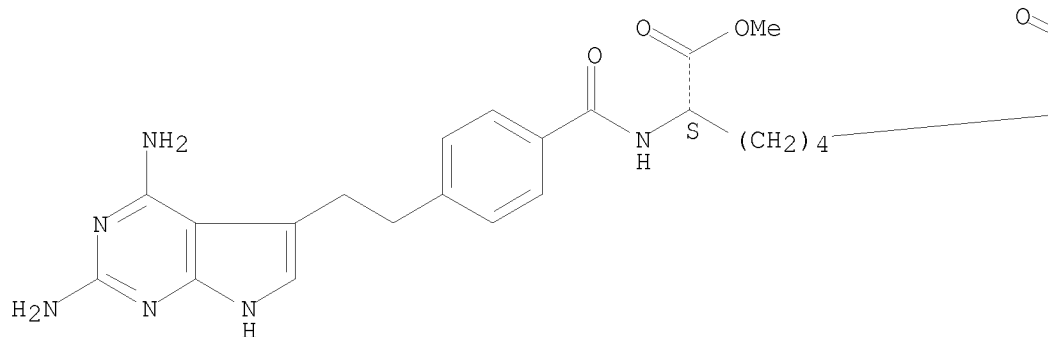


RN 303957-87-1 CAPLUS

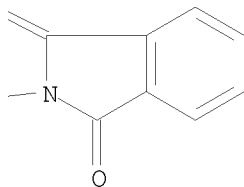
CN 2H-Isoindole-2-hexanoic acid,  $\alpha$ -[[4-[2-(2,4-diamino-1H-pyrrolo[2,3-d]pyrimidin-5-yl)ethyl]benzoyl]amino]-1,3-dihydro-1,3-dioxo-, methyl ester, ( $\alpha$ S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A



PAGE 1-B



RE.CNT 29 THERE ARE 29 CITED REFERENCES AVAILABLE FOR THIS RECORD  
ALL CITATIONS AVAILABLE IN THE RE FORMAT

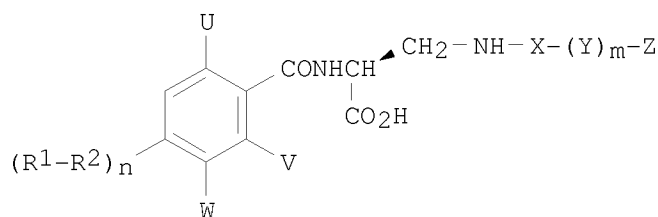
L6 ANSWER 12 OF 22 CAPLUS COPYRIGHT 2007 ACS on STN  
AN 2000:260225 CAPLUS  
DN 132:294010  
TI Preparation of diaminopropionic acid derivatives as intracellular adhesion  
molecule-1 (ICAM-1) binding inhibitors  
IN Fotouhi, Nader; Gillespie, Paul; Guthrie, Robert William; Pietranico-Cole,  
Sherrie Lynn; Yun, Weiya  
PA F. Hoffmann-La Roche A.-G., Switz.  
SO PCT Int. Appl., 259 pp.  
CODEN: PIXXD2

DT Patent  
LA English

FAN.CNT 1

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2000021920	A1	20000420	WO 1999-EP7620	19991012
W:				
AE, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CU, CZ,				
DE, DK, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS,				
JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG,				
MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL,				
TJ, TM, TR, TT, UA, UG, UZ, VN, YU, ZA, ZW				
RW:				
GH, GM, KE, LS, MW, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE,				
DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF,				
CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG				
US 6331640	B1	20011218	US 1999-407534	19990929
CA 2344058	A1	20000420	CA 1999-2344058	19991012

BR 9914602	A	20010703	BR 1999-14602	19991012
EP 1121342	A1	20010808	EP 1999-953772	19991012
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO				
TR 200101038	T2	20010921	TR 2001-1038	19991012
JP 2002527416	T	20020827	JP 2000-575829	19991012
JP 3720709	B2	20051130		
AU 766468	B2	20031016	AU 2000-10349	19991012
MX 2001PA03284	A	20011011	MX 2001-PA3284	20010329
ZA 2001002608	A	20020930	ZA 2001-2608	20010329
US 2002052512	A1	20020502	US 2001-879700	20010612
US 2004006236	A1	20040108	US 2003-349289	20030122
US 6803384	B2	20041012		
US 2005080119	A1	20050414	US 2004-945650	20040921
US 7217728	B2	20070515		
US 2007155671	A1	20070705	US 2007-703925	20070208
PRAI US 1998-104120P	P	19981013		
US 1999-407534	A3	19990929		
WO 1999-EP7620	W	19991012		
US 2001-879700	B3	20010612		
US 2003-349289	A3	20030122		
US 2004-945650	A3	20040921		
OS	MARPAT 132:294010			
GI				

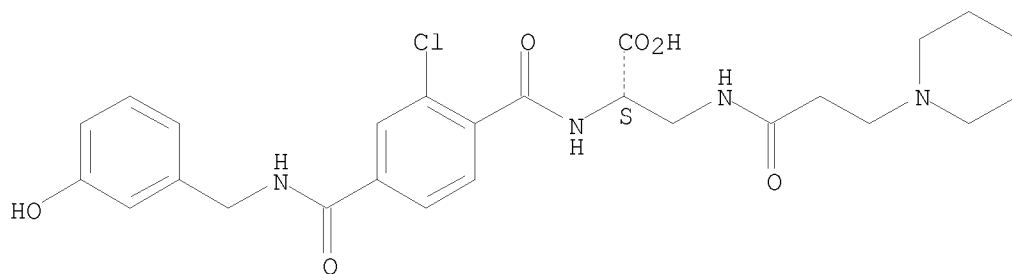


AB Diaminopropionic acid derivs. I [R1 = substituted 1-naphthyl, 4-indolyl, 4-benzimidazolyl, 4-benzodiazolyl, 4-benzotriazolyl, or phenyl; R2 = CHR3NHCO (R3 = H, carboxy, alkyl), CH2CH2CO, 1,2-cyclopropanediylcarbonyl, OCH2CO, CH:CHCHR3, CH2CH2CH(OH), CONHCHR3, or CH2NH-5,1-tetrazolediyl; U, V, W = H, halo, alkyl provided that U and V are not both hydrogen; X = CO, phenylalkylene, sulfonyl; Y = alkylene which may be substituted by amino or cycloalkyl, alkenylene, alkyleneethio; Z = H, alkylthio, CO2H, CONH2, 1-adamantyl, diphenylmethyl, 3-[[[(5-chloro-2-pyridinyl)amino]carbonyl]-2-pyrazinyl, hydroxy, phenylmethoxy, 2-chloro-4-[[[(3-hydroxyphenyl)methyl]amino]carbonyl]phenyl, [(2,6-dichlorophenyl)methoxy], Ph, (un)substituted cycloalkyl or aryl or fused ring system which may contain 0-3 heteroatoms; m, n = 0, 1] or their pharmaceutically acceptable salts or esters were prepared and are useful for treating rheumatoid arthritis, psoriasis, multiple sclerosis, Crohn's disease, ulcerative colitis, atherosclerosis, restenosis, pancreatitis, transplant rejection, delayed graft function and diseases of ischemia reperfusion injury, including acute myocardial infarction and stroke. Thus, N-[2-chloro-4-[[[(3-hydroxyphenyl)methyl]amino]carbonyl]benzoyl]-3-(3-methoxybenzoylamino)-L-alanine was prepared by the solid-phase method and showed IC50 = 1.2 nM in the LFA-1 (lymphocyte function-associated



antigen-1)/ICAM-1 protein-protein assay.  
 IT 264273-57-6P  
 RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)  
 (preparation of diaminopropionic acid derivs. as intracellular adhesion mol.-1 (ICAM-1) binding inhibitors)  
 RN 264273-57-6 CAPLUS  
 CN L-Alanine, N-[2-chloro-4-[[[(3-hydroxyphenyl)methyl]amino]carbonyl]benzoyl]-3-[[1-oxo-3-(1-piperidiny)propyl]amino]- (CA INDEX NAME)

Absolute stereochemistry.



RE.CNT 3 THERE ARE 3 CITED REFERENCES AVAILABLE FOR THIS RECORD  
 ALL CITATIONS AVAILABLE IN THE RE FORMAT

L6 ANSWER 13 OF 22 CAPLUS COPYRIGHT 2007 ACS on STN  
 AN 2000:175829 CAPLUS  
 DN 132:208143  
 TI Preparation of peptides as NK-1 receptor antagonists  
 IN Groger, Karsten; Sisto, Alessandro  
 PA Menarini Ricerche S.p.A., Italy  
 SO PCT Int. Appl., 43 pp.  
 CODEN: PIXXD2

DT Patent  
 LA English

FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 2000014109	A1	20000316	WO 1999-EP6541	19990906
	W:	AE, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CR, CU, CZ, DE, DK, DM, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM			
	RW:	GH, GM, KE, LS, MW, SD, SL, SZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG			
	IT 1304898	B1	20010405	IT 1998-FI201	19980908
	AU 9957457	A1	20000327	AU 1999-57457	19990906
PRAI	IT 1998-FI201	A	19980908		
	WO 1999-EP6541	W	19990906		
OS	MARPAT 132:208143				
AB	Peptides R1(CH2)nCONHCH[(CH2)pR2]CONHCHR3CONR4R5 [(S)-configuration at				

CHR3; n = 0-3; p = 0-4; R1 = a basic moiety chosen from an amino or heterocyclyl group, aryl or arylalkyl which can be substituted on the aromatic moiety; R2 = R6(CH<sub>2</sub>)<sub>m</sub>-X1-, where m = 0-3; R6 = amino group, heterocyclyl, aryl or arylalkyl which can be substituted on the aromatic moiety; X1 = CONH or NHC=O; R3 = naphthylmethyl, halobenzyl, indolylmethyl; R4 = aryl or arylalkyl which can be substituted on the aromatic moiety; R5 = H, Me] (with provisos) were prepared as NK-1 receptor antagonists. Thus, Na-{Na-[(1H)indol-3-ylcarbonyl]-L-asparaginyl[β-N-[2-(morpholin-4-yl)ethyl]]}-L-[3-(3,4-dichlorophenyl)alanine]-N-methyl-N-(4-bromobenzyl)amide, prepared by step-wise couplings in solution, showed pK<sub>i</sub> = 9.3 for inhibition of [3H]SP binding to IM9 cells.

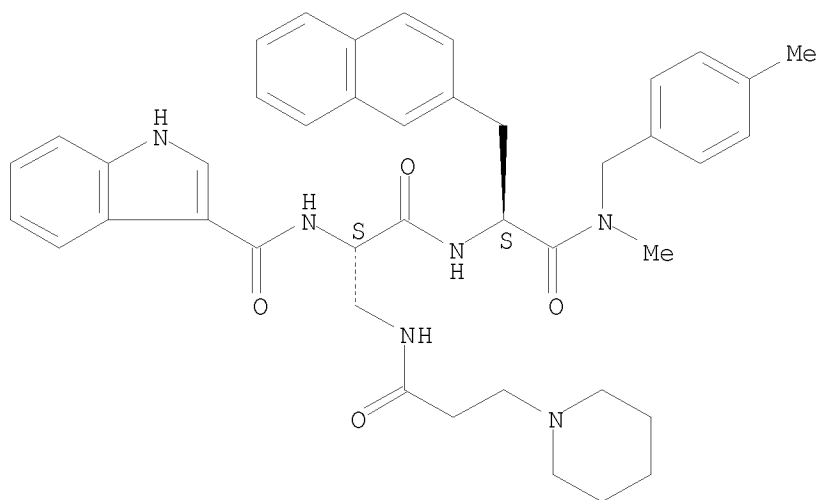
IT 260809-08-3P 260809-12-9P 260809-13-0P  
260809-14-1P 260809-16-3P 260809-17-4P  
260809-18-5P

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)  
(preparation of peptides as NK-1 receptor antagonists)

RN 260809-08-3 CAPLUS

CN L-Alaninamide, N-(1H-indol-3-ylcarbonyl)-3-[[1-oxo-3-(1-piperidinyl)propyl]amino]-L-alanyl-N-methyl-N-[(4-methylphenyl)methyl]-3-(2-naphthalenyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

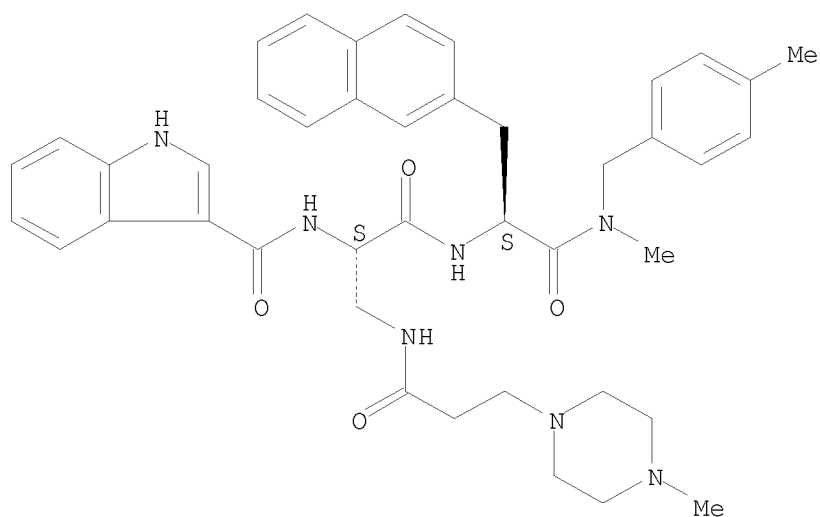


RN 260809-12-9 CAPLUS

CN L-Alaninamide, N-(1H-indol-3-ylcarbonyl)-3-[[3-(4-methyl-1-piperazinyl)-1-oxopropyl]amino]-L-alanyl-N-methyl-N-[(4-methylphenyl)methyl]-3-(2-naphthalenyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

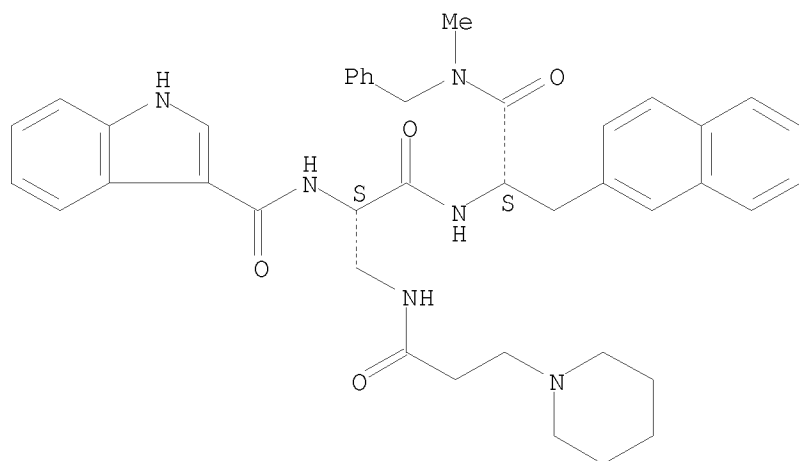
10/539372



RN 260809-13-0 CAPLUS

CN L-Alaninamide, N-(1H-indol-3-ylcarbonyl)-3-[[1-oxo-3-(1-piperidinyl)propyl]amino]-L-alanyl-N-methyl-3-(2-naphthalenyl)-N-(phenylmethyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

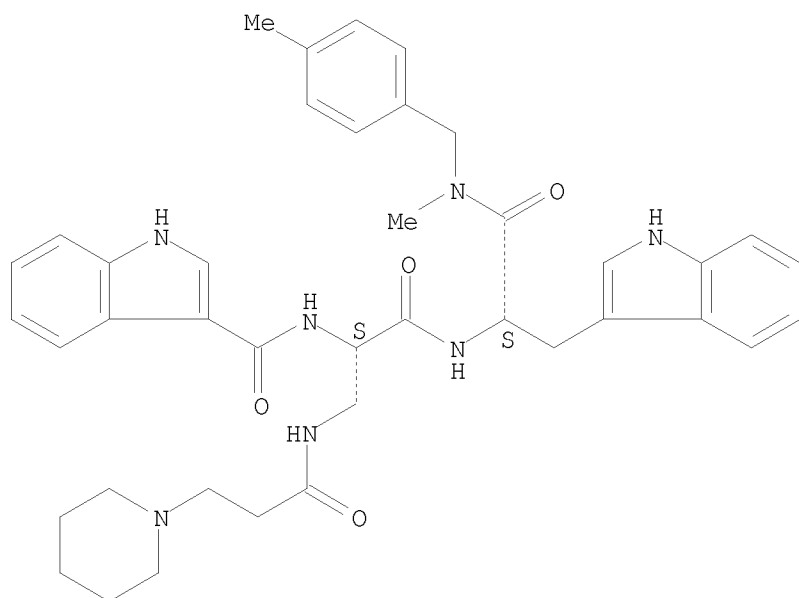


RN 260809-14-1 CAPLUS

CN L-Tryptophanamide, N-(1H-indol-3-ylcarbonyl)-3-[[1-oxo-3-(1-piperidinyl)propyl]amino]-L-alanyl-N-methyl-N-[(4-methylphenyl)methyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

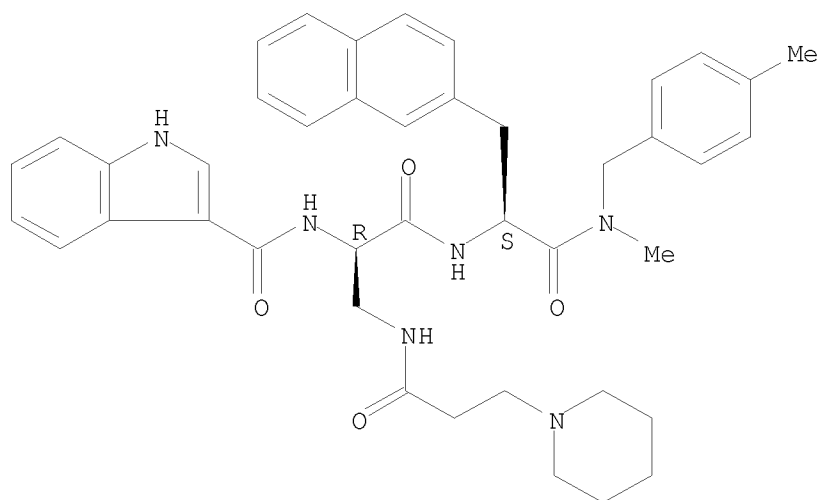
10/539372



RN 260809-16-3 CAPLUS

CN L-Alaninamide, N-(1H-indol-3-ylcarbonyl)-3-[[1-oxo-3-(1-piperidinyl)propyl]amino]-D-alanyl-N-methyl-N-[(4-methylphenyl)methyl]-3-(2-naphthalenyl)- (9CI) (CA INDEX NAME)

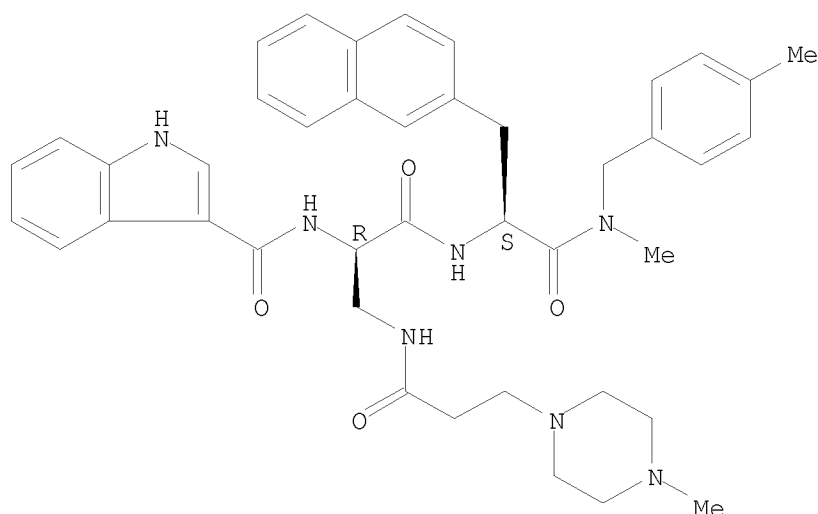
Absolute stereochemistry.



RN 260809-17-4 CAPLUS

CN L-Alaninamide, N-(1H-indol-3-ylcarbonyl)-3-[[3-(4-methyl-1-piperazinyl)-1-oxopropyl]amino]-D-alanyl-N-methyl-N-[(4-methylphenyl)methyl]-3-(2-naphthalenyl)- (9CI) (CA INDEX NAME)

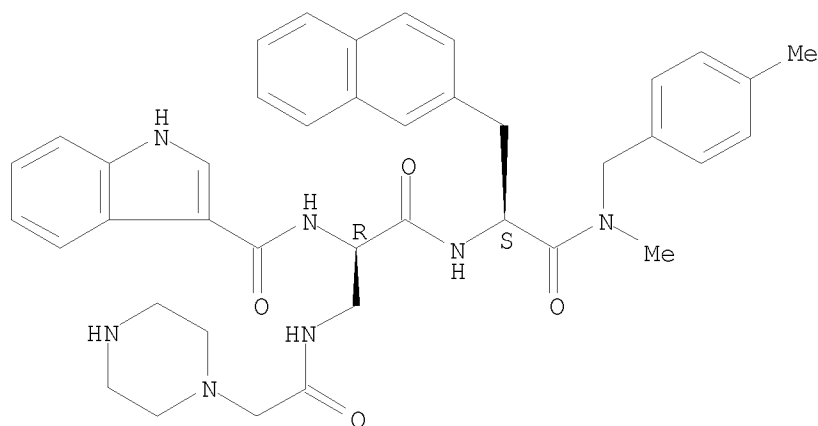
Absolute stereochemistry.



RN 260809-18-5 CAPLUS

CN L-Alaninamide, N-(1H-indol-3-ylcarbonyl)-3-[(1-piperazinylacetyl)amino]-D-alanyl-N-methyl-N-[(4-methylphenyl)methyl]-3-(2-naphthalenyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RE.CNT 3 THERE ARE 3 CITED REFERENCES AVAILABLE FOR THIS RECORD  
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L6 ANSWER 14 OF 22 CAPLUS COPYRIGHT 2007 ACS on STN

AN 1997:53583 CAPLUS

DN 126:70149

TI Hydrochlorides of 1-phenyl-1-(p-nitrobenzoyl amino)-5-(n-piperidino)- or (n-diethylamino)pentanes having antiarrhythmic and antifibrillation activity

IN Mashkovskij, M. D.; Glushkov, R. G.; Skachilova, S. Ya.; Dorodnikova, E. V.; Rozenshtaukh, L. V.; Voronin, V. G.; Zheltukhin, N. K.; Anyukhovskij, E. P.; Nesterenko, V. V.; Cherkasova, E. M.

PA Tsentr Po Khimii Lekarstvennykh Sredstv, USSR; Vsesoyuznyj Nauchnyj Tsentr  
Po Bezopasnosti Biologicheskii Aktivnykh Veshchestv; Vsesoyuznyj  
Kardiologicheskij Nauchnyj Tsentr Amn Sssr

SO U.S.S.R.

From: Izobreteniya 1996, (6), 261.

CODEN: URXXAF

DT Patent

LA Russian

FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	SU 1833612	A3	19960227	SU 1987-4359472	19871208
PRAI	SU 1987-4359472		19871208		

AB Title only translated.

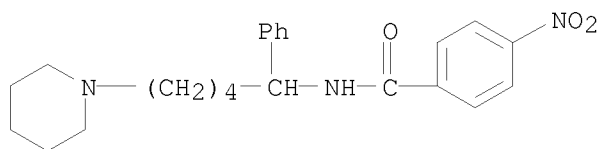
IT 185384-75-2

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); THU (Therapeutic use); BIOL (Biological study); USES (Uses)

(Hydrochlorides of 1-phenyl-1-(p-nitrobenzoyl amino)-5-(n-piperidino)- or (n-diethylamino)pentanes having antiarrhythmic and antifibrillation activity)

RN 185384-75-2 CAPLUS

CN Benzamide, 4-nitro-N-[1-phenyl-5-(1-piperidinyl)pentyl]-, monohydrochloride (9CI) (CA INDEX NAME)



● HCl

L6 ANSWER 15 OF 22 CAPLUS COPYRIGHT 2007 ACS on STN

AN 1996:494173 CAPLUS

DN 125:143330

TI Peptide compounds for prevention and/or treatment of nitric oxide (NO)-mediated diseases

IN Itoh, Yoshikuni; Iwamoto, Toshiro; Yatabe, Takumi; Hamashima, Hitoshi; Inoue, Takayuki; Hashimoto, Seiji; Oku, Teruo

PA Fujisawa Pharmaceutical Co., Ltd., Japan

SO PCT Int. Appl., 739 pp.

CODEN: PIXXD2

DT Patent

LA English

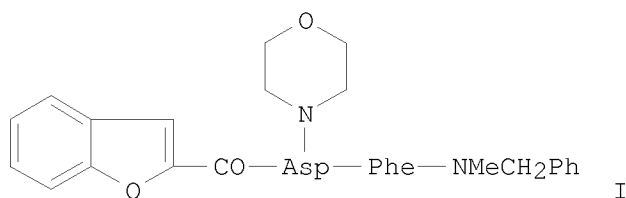
FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 9616981	A2	19960606	WO 1995-JP2428	19951129
	WO 9616981	A3	19960906		

W: AU, CA, CN, FI, HU, JP, KR, MX, NO, NZ, RU, UA, US

RW: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE,  
 BF, BJ, CF, CG, CI, CM, GA, GN, ML, MR, NE, SN, TD, TG

AU 9539937	A	19960619	AU 1995-39937	19951129
EP 796270	A2	19970924	EP 1995-938602	19951129
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LI, LU, NL, PT, SE				
ZA 9510201	A	19960625	ZA 1995-10201	19951130
US 5932737	A	19990803	US 1997-849076	19970530
PRAI GB 1994-24408	A	19941202		
GB 1995-4891	A	19950310		
GB 1995-10042	A	19950518		
WO 1995-JP2428	W	19951129		
OS MARPAT 125:143330				
GI				



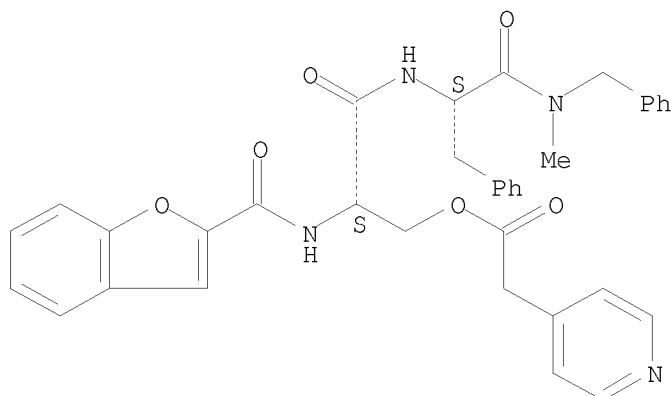
AB Peptides WA1NR8CH(A2T)CONR9CH(A3R3)R4 [W = alkyl, (un)substituted aryl or fluorenyl, etc.; A1 = alkylene, NHCO, CO, CS, SO2; A2 = alkylene; T = H, aryl, heterocyclyl, OH, etc.; R8 = H, alkyl; R8 may link with A2T to form CH2C6H4CH2-o (Q); A3 = bond, alkylene; R3 = H, aryl, OH, etc.; R9 = H, alkyl or may link with A3R3 to form Q; R4 = CO2H, protected carboxy, carboxamido, etc. or CH(A3R3)R4 = N-alkyl-2-oxoquinoline moiety] or their pharmaceutically acceptable salts were prepared for use as medicaments. Thus, dipeptide I was prepared by acylation of aspartylphenylalaninamide derivative with 2-benzofurancarboxylic acid. I and six other peptides showed 100% inhibition of NO production in tests of murine macrophage cells.

IT 179881-40-4P 179881-43-7P  
 RL: SPN (Synthetic preparation); PREP (Preparation)  
 (preparation of peptides for prevention and/or treatment of nitric oxide-mediated diseases)

RN 179881-40-4 CAPLUS

CN L-Phenylalaninamide, N-(2-benzofuranylcabonyl)-O-(4-pyridinylacetyl)-L-seryl-N-methyl-N-(phenylmethyl)- (9CI) (CA INDEX NAME)

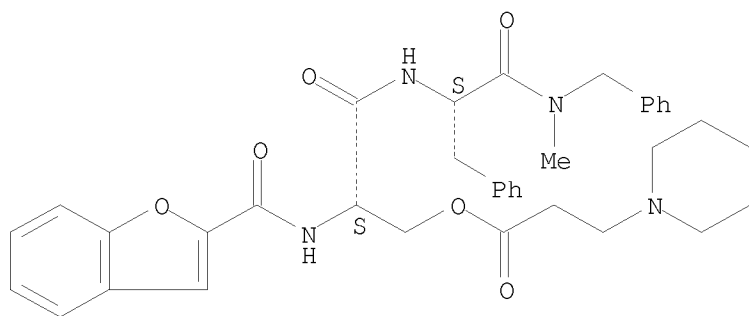
Absolute stereochemistry.



RN 179881-43-7 CAPLUS

CN L-Phenylalaninamide, N-(2-benzofuranylcarbonyl)-O-[1-oxo-3-(1-piperidinyl)propyl]-L-seryl-N-methyl-N-(phenylmethyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L6 ANSWER 16 OF 22 CAPLUS COPYRIGHT 2007 ACS on STN

AN 1995:904875 CAPLUS

DN 124:240

TI Search for antiarrhythmic drugs among 1,5-diaminopentane derivatives

AU Mashkovskii, M. D.; Glushkov, R. G.; Dorodnikova, E. V.; Yuzhakov, S. D.

CS TSKhLS, VNIKhFI, Moscow, Russia

SO Khimiko-Farmatsevticheskii Zhurnal (1995), 29(3), 27-31

CODEN: KHFZAN; ISSN: 0023-1134

PB Meditsina

DT Journal

LA Russian

AB Most of the 28 1,5-diaminopentanes tested showed antiarrhythmic activity in rats. Structure-activity relations are briefly discussed.

IT 171203-85-3 171203-86-4 171203-87-5

171203-88-6 171203-89-7 171203-90-0

171203-91-1 171203-92-2 171203-93-3

171203-94-4 171203-95-5 171203-96-6

171203-99-9 171204-00-5 171204-01-6

171204-02-7 171204-03-8 171204-04-9



10/539372

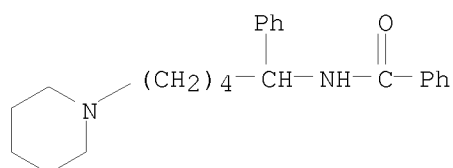
171204-05-0 171204-06-1 171204-07-2

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); PRP (Properties); THU (Therapeutic use); BIOL (Biological study); USES (Uses)

(search for antiarrhythmic drugs among 1,5-diaminopentane derivs.)

RN 171203-85-3 CAPLUS

CN Benzamide, N-[1-phenyl-5-(1-piperidinyl)pentyl]- (CA INDEX NAME)



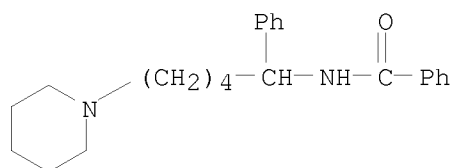
RN 171203-86-4 CAPLUS

CN 3-Pyridinecarboxylic acid, compd. with N-[1-phenyl-5-(1-piperidinyl)pentyl]benzamide (1:1) (9CI) (CA INDEX NAME)

CM 1

CRN 171203-85-3

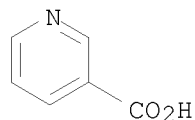
CMF C23 H30 N2 O



CM 2

CRN 59-67-6

CMF C6 H5 N O2



RN 171203-87-5 CAPLUS

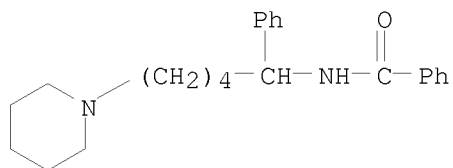
CN 4-Pyrimidinecarboxylic acid, 1,2,3,6-tetrahydro-2,6-dioxo-, compd. with N-[1-phenyl-5-(1-piperidinyl)pentyl]benzamide (1:1) (CA INDEX NAME)

CM 1

CRN 171203-85-3

CMF C23 H30 N2 O

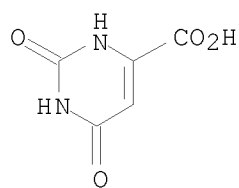
10/539372



CM 2

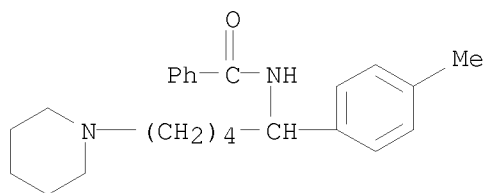
CRN 65-86-1

CMF C5 H4 N2 O4



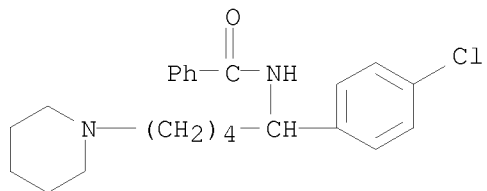
RN 171203-88-6 CAPLUS

CN Benzamide, N-[1-(4-methylphenyl)-5-(1-piperidinyl)pentyl]- (CA INDEX NAME)



RN 171203-89-7 CAPLUS

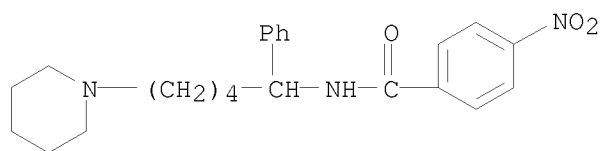
CN Benzamide, N-[1-(4-chlorophenyl)-5-(1-piperidinyl)pentyl]- (CA INDEX NAME)



RN 171203-90-0 CAPLUS

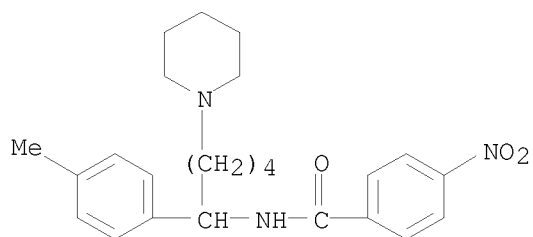
CN Benzamide, 4-nitro-N-[1-phenyl-5-(1-piperidinyl)pentyl]- (CA INDEX NAME)

10/539372



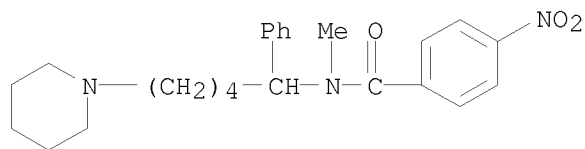
RN 171203-91-1 CAPLUS

CN Benzamide, N-[1-(4-methylphenyl)-5-(1-piperidinyl)pentyl]-4-nitro- (CA INDEX NAME)



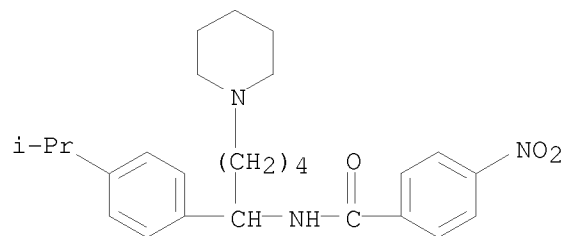
RN 171203-92-2 CAPLUS

CN Benzamide, N-methyl-4-nitro-N-[1-phenyl-5-(1-piperidinyl)pentyl]- (CA INDEX NAME)



RN 171203-93-3 CAPLUS

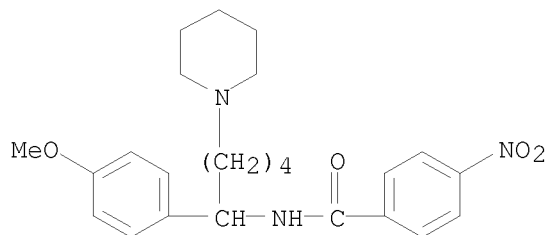
CN Benzamide, N-[1-[4-(1-methylethyl)phenyl]-5-(1-piperidinyl)pentyl]-4-nitro- (CA INDEX NAME)



RN 171203-94-4 CAPLUS

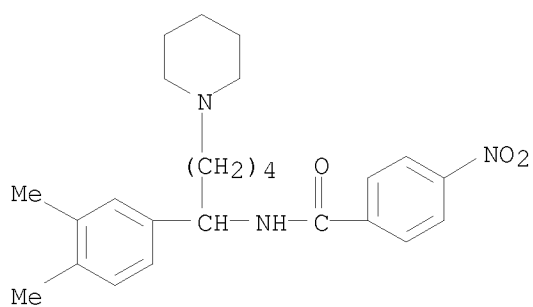
CN Benzamide, N-[1-(4-methoxyphenyl)-5-(1-piperidinyl)pentyl]-4-nitro- (CA INDEX NAME)

10/539372



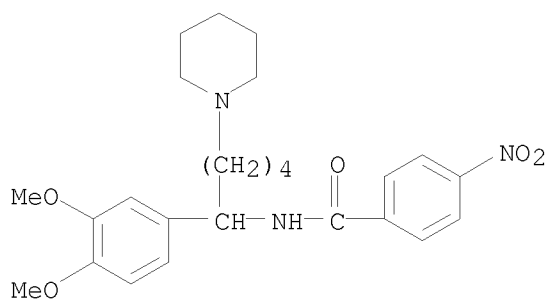
RN 171203-95-5 CAPLUS

CN Benzamide, N-[1-(3,4-dimethylphenyl)-5-(1-piperidinyl)pentyl]-4-nitro-  
(CA INDEX NAME)



RN 171203-96-6 CAPLUS

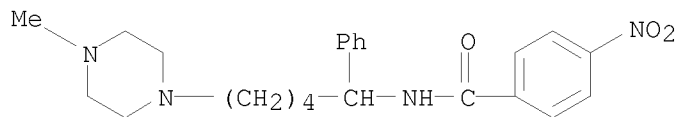
CN Benzamide, N-[1-(3,4-dimethoxyphenyl)-5-(1-piperidinyl)pentyl]-4-nitro-  
(CA INDEX NAME)



RN 171203-99-9 CAPLUS

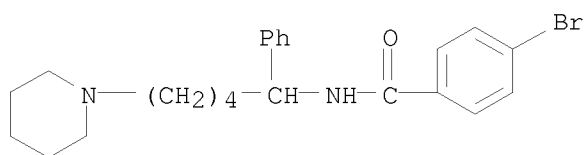
CN Benzamide, N-[5-(4-methyl-1-piperazinyl)-1-phenylpentyl]-4-nitro-,  
dihydrochloride (9CI) (CA INDEX NAME)

10/539372

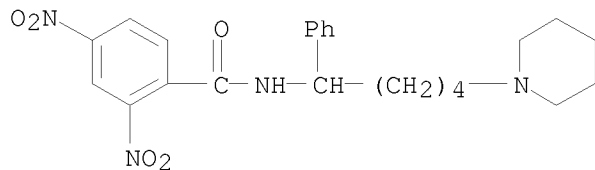


● 2 HCl

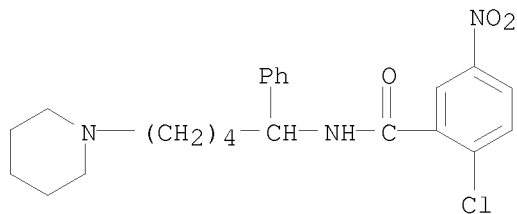
RN 171204-00-5 CAPLUS  
CN Benzamide, 4-bromo-N-[1-phenyl-5-(1-piperidinyl)pentyl]- (CA INDEX NAME)



RN 171204-01-6 CAPLUS  
CN Benzamide, 2,4-dinitro-N-[1-phenyl-5-(1-piperidinyl)pentyl]- (CA INDEX NAME)

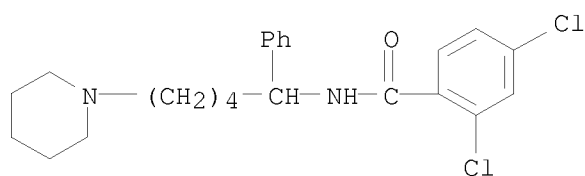


RN 171204-02-7 CAPLUS  
CN Benzamide, 2-chloro-5-nitro-N-[1-phenyl-5-(1-piperidinyl)pentyl]- (CA INDEX NAME)



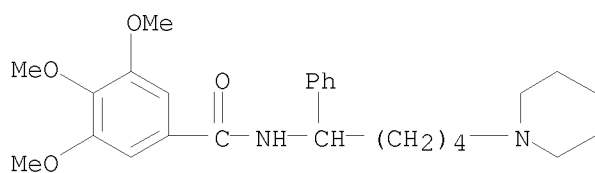
RN 171204-03-8 CAPLUS  
CN Benzamide, 2,4-dichloro-N-[1-phenyl-5-(1-piperidinyl)pentyl]- (CA INDEX NAME)

10/539372



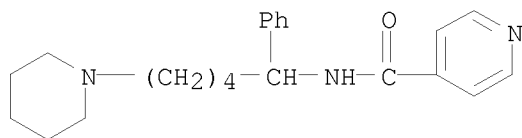
RN 171204-04-9 CAPLUS

CN Benzamide, 3,4,5-trimethoxy-N-[1-phenyl-5-(1-piperidinyl)pentyl]- (CA INDEX NAME)



RN 171204-05-0 CAPLUS

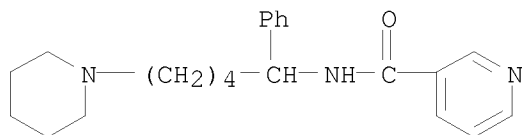
CN 4-Pyridinecarboxamide, N-[1-phenyl-5-(1-piperidinyl)pentyl]-, dihydrochloride (9CI) (CA INDEX NAME)



● 2 HCl

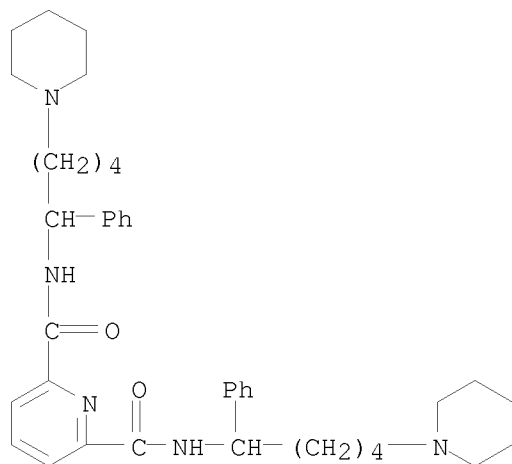
RN 171204-06-1 CAPLUS

CN 3-Pyridinecarboxamide, N-[1-phenyl-5-(1-piperidinyl)pentyl]- (CA INDEX NAME)

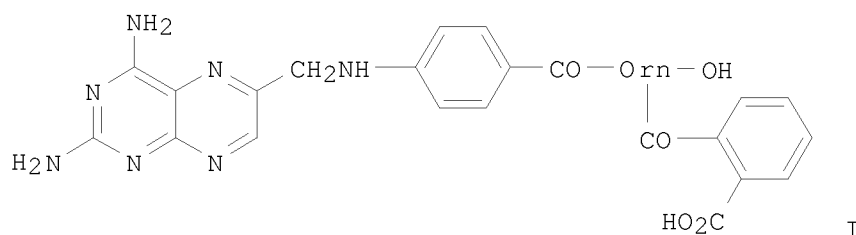


RN 171204-07-2 CAPLUS

CN 2,6-Pyridinedicarboxamide, N,N'-bis[1-phenyl-5-(1-piperidinyl)pentyl]- (9CI) (CA INDEX NAME)



L6 ANSWER 17 OF 22 CAPLUS COPYRIGHT 2007 ACS on STN  
 AN 1994:605936 CAPLUS  
 DN 121:205936  
 TI Synthesis and Biological Activity of N $\alpha$ -Hemiphthaloyl-  
 $\alpha,\omega$ -diaminoalkanoic Acid Analogs of Aminopterin and  
 3',5-Dichloroaminopterin  
 AU Rosowsky, Andre; Bader, Henry; Wright, Joel E.; Keyomarsi, Khandan;  
 Matherly, Larry H.  
 CS Dana-Farber Cancer Institute, Harvard Medical School, Boston, MA, 02115,  
 USA  
 SO Journal of Medicinal Chemistry (1994), 37(14), 2167-74  
 CODEN: JMCMAR; ISSN: 0022-2623  
 DT Journal  
 LA English  
 GI



AB Analogs of N $\alpha$ -(4-amino-4-deoxypteroyl)-N $\delta$ -(hemiphthaloyl)-L-  
 ornithine (I) (PT523) with 3',5'-dichloro substitution in the  
 p-aminobenzoyl moiety or with one less or more CH<sub>2</sub> group in the amino acid  
 moiety were synthesized and tested as inhibitors of dihydrofolate  
 reductase (DHFR) activity and cell growth. Replacement of L-ornithine in  
 I by L-2,4-diaminobutanoic acid or L-lysine did not decrease binding to  
 human recombinant DHFR but resulted in some loss of activity against SCC25  
 human and SCC VII murine squamous cell carcinoma and against MCF-7 human  
 breast carcinoma in culture. PT523 was several times more potent than

methotrexate (MTX), aminopterin (AMT), or trimetrexate (TMQ). 3',5'-Dichloro substitution did not decrease either DHFR binding or cytotoxicity. A new synthetic route to I from 2,4-diamino-6-(hydroxymethyl)pteridine and N $\alpha$ -(4-aminobenzoyl)-N $\delta$ -phthaloyl-L-ornithine Me ester was investigated but was not superior to previously described methods. In comparative expts. on the ability of PT523 and MTX to competitively inhibit the influx of (6R)-5,10-dideazatetrahydrofolate (DDATHF, lometrexol), used a surrogate for MTX and reduced folates, the K<sub>i</sub> of PT523 was lower than that of MTX in both wild-type CCRF-CEM human leukemic lymphoblasts and the transport- and polyglutamylation-defective subline CEM/MTX. The CCRF-CEM cells were 10-fold more sensitive to PT523 than to MTX, whereas the CEM/MTX cells were 240-fold more sensitive. However, in contrast to other MTX-resistant cells where collateral sensitivity to PT523 has been seen. CEM/MTX cells still showed substantial cross resistance to PT523 which may reflect an unusual heightened ability to utilize exogenous folic acid. The good correlation observed with both cell lines between the cytotoxicity of PT523 and MTX and the ability to inhibit DDATHF influx supported the view that PT523 and MTX share, at least in part, a common protein carrier for membrane transport.

IT 158090-66-5P

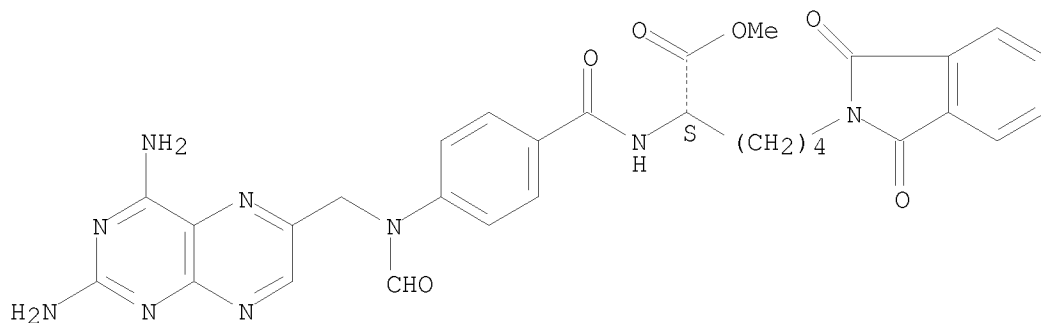
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation, saponification, and imide ring opening of)

RN 158090-66-5 CAPLUS

CN 2H-Isoindole-2-hexanoic acid,  $\alpha$ -[[4-[[[(2,4-diamino-6-pteridinyl)methyl]formylamino]benzoyl]amino]-1,3-dihydro-1,3-dioxo-, methyl ester, (S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L6 ANSWER 18 OF 22 CAPLUS COPYRIGHT 2007 ACS on STN

AN 1993:626417 CAPLUS

DN 119:226417

TI Preparation of condensed pyrimidinylacyl amino acids as neoplasm inhibitors

IN Akimoto, Hiroshi; Ootsu, Koichiro; Itoh, Fumio

PA Takeda Chemical Industries, Ltd., Japan

SO Eur. Pat. Appl., 51 pp.

CODEN: EPXXDW

DT Patent

LA English

FAN.CNT 1

PATENT NO.

KIND

DATE

APPLICATION NO.

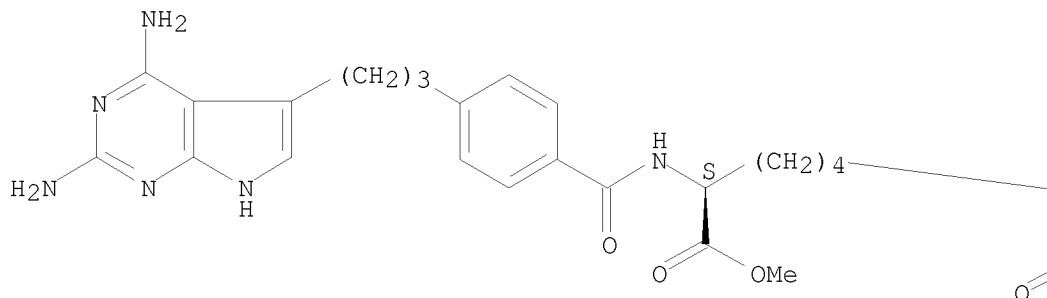
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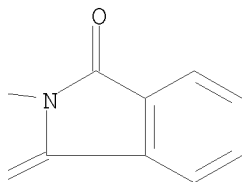


PI	EP 530537	A1	19930310	EP 1992-113523	19920807
	EP 530537	B1	19970108		
	R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LI, LU, NL, PT, SE				
	US 5403843	A	19950404	US 1992-926170	19920807
	AT 147386	T	19970115	AT 1992-113523	19920807
	CA 2075787	A1	19930213	CA 1992-2075787	19920811
	JP 06049069	A	19940222	JP 1992-214142	19920811
	JP 3376479	B2	20030210		
PRAI	JP 1991-202042	A	19910812		
	JP 1992-71513	A	19920327		
	JP 1992-145851	A	19920605		
OS	CASREACT 119:226417; MARPAT 119:226417				
GI	For diagram(s), see printed CA Issue.				
AB	<p>Title compds. [I; ring A = (substituted) (hydrogenated) 5-membered ring; B = (substituted) divalent 5- or 6-membered homo- or heterocyclic group; X = amino, OH, SH; Y = H, halo, C-, N-, O-, or S-bonded group; Z = (substituted) (heteroatom-containing) divalent group having ≤5 atoms; W = NRCO; R = H, (substituted) alkyl; R1 = (substituted) cyclic or chain-like group; or RR1 = atoms to form a 3-13 membered ring CO2R2 = optionally esterified carboxyl group; p = 1-4; with provisos], were prepared Thus, Nα-[4-[2-(2,4-diamino-7H-pyrrolo[2,3-d]pyrimidin-5-yl)ethyl]benzoyl]-Nδ-phthaloyl-L-ornithine Me ester [prepared by condensation of the corresponding benzoic acid with Nδ-phthaloyl-L-ornithine Me ester.HCl using di-Et cyanophosphate and Et3N in DMF] was saponified to give Nα-[4-[2-(2,4-diamino-7H-pyrrolo[2,3-d]pyrimidin-5-yl)ethyl]benzoyl]-Nδ-hemiphthaloyl-L-ornithine. This inhibited proliferation of A549 cells with IC50 = 0.0012 μg/mL.</p>				
IT	<p>149009-83-6P          RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)          (preparation of, as neoplasm inhibitor)</p>				
RN	149009-83-6 CAPLUS				
CN	<p>2H-Isindole-2-hexanoic acid, α-[[4-[3-(2,4-diamino-1H-pyrrolo[2,3-d]pyrimidin-5-yl)propyl]benzoyl]amino]-1,3-dihydro-1,3-dioxo-, methyl ester, (αS)- (9CI) (CA INDEX NAME)</p>				

Absolute stereochemistry.

PAGE 1-A





L6 ANSWER 19 OF 22 CAPLUS COPYRIGHT 2007 ACS on STN  
 AN 1993:603167 CAPLUS  
 DN 119:203167  
 TI Substituted 1-phenyl-1-benzoylamino-5-aminopentanes, their preparation and use  
 IN Mashkovsky, Mikhail D.; Glushkov, Robert G.; Skachilova, Sofiya Y.; Dorodnikova, Elena V.; Rosenshtraukh, Leonid V.; Voronin, Vasily G.; Zheltukhin, Nikolai K.; Anjukhovskiy, Evgenii P.; Nesterenko, Vladislav V.; et al.  
 PA USSR  
 SO Can. Pat. Appl., 12 pp.  
 CODEN: CPXXEB  
 DT Patent  
 LA English  
 FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	CA 2073833	A1	19930301	CA 1992-2073833	19920714
	EP 535256	A1	19930407	EP 1991-114635	19910830
	R: AT, BE, CH, DE, DK, ES, FR, GB, IT, LI, NL, SE				
	HU 62854	A2	19930628	HU 1992-2316	19920714
	ZA 9205237	A	19940114	ZA 1992-5237	19920714
	AU 9220407	A	19930304	AU 1992-20407	19920720
	AU 648422	B2	19940421		
	BR 9202849	A	19930406	BR 1992-2849	19920723
	JP 06192197	A	19940712	JP 1992-226829	19920826
PRAI	EP 1991-114635	A	19910830		
OS	CASREACT 119:203167; MARPAT 119:203167				
GI					



I

AB The title compds. (I; R1 = halo, NO2, C1-4 aminoacyl, sulfonamido; R2, R3 = C1-5 alkyl or R2R3 = C3-6 alkylene) and their optically active isomers and their physiol. tolerated acids are prepared as antiarrhythmic and

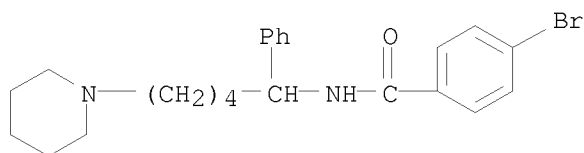
antifibrillatory compds. [e.g., (+)-I (R1 = p-NO<sub>2</sub>, R2 = R3 = Et).HCl [(±)-II]; (+)- and (-)-II]. Thus, Et<sub>2</sub>N(CH<sub>2</sub>)<sub>4</sub>CH(NH<sub>2</sub>)Ph.HCl in 10% aqueous NaOH-Me<sub>2</sub>CO is treated with p-O<sub>2</sub>NC<sub>6</sub>H<sub>4</sub>COCl to give I (R1 = p-NO<sub>2</sub>, R2 = R3 = Et); this in Me<sub>2</sub>CO with HCl in Me<sub>2</sub>CHOH gives (±)-II. Dosages are given.

IT 150492-00-5 150492-01-6 185384-75-2

RL: RCT (Reactant); RACT (Reactant or reagent)  
(preparation as antiarrhythmic)

RN 150492-00-5 CAPLUS

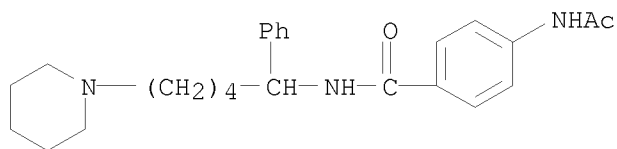
CN Benzamide, 4-bromo-N-[1-phenyl-5-(1-piperidinyl)pentyl]-,  
monohydrochloride (9CI) (CA INDEX NAME)



● HCl

RN 150492-01-6 CAPLUS

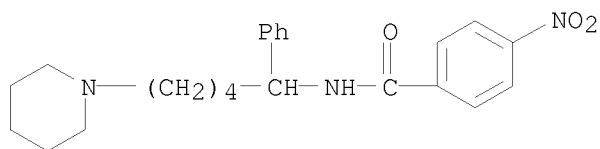
CN Benzamide, 4-(acetylamino)-N-[1-phenyl-5-(1-piperidinyl)pentyl]-,  
monohydrochloride (9CI) (CA INDEX NAME)



● HCl

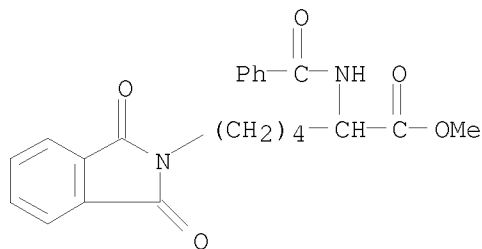
RN 185384-75-2 CAPLUS

CN Benzamide, 4-nitro-N-[1-phenyl-5-(1-piperidinyl)pentyl]-,  
monohydrochloride (9CI) (CA INDEX NAME)



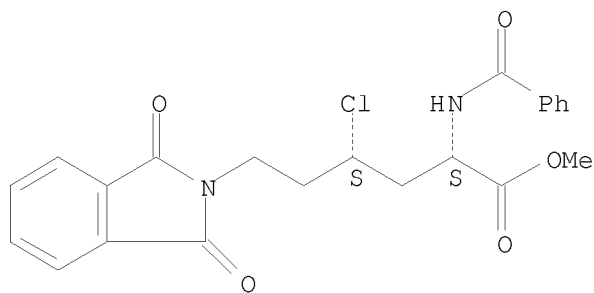
● HCl

L6 ANSWER 20 OF 22 CAPLUS COPYRIGHT 2007 ACS on STN  
 AN 1991:229364 CAPLUS  
 DN 114:229364  
 TI Synthesis of  $\alpha,\omega$ -diamino acids via amidocarbonylation  
 reaction: novel synthesis of lysine, ornithine, and their analogs.  
 AU Amino, Yusuke; Izawa, Kunisuke  
 CS Cent. Res. Lab., Ajinomoto Co., Inc., Kawasaki, 210, Japan  
 SO Bulletin of the Chemical Society of Japan (1991), 64(2), 613-19  
 CODEN: BCSJA8; ISSN: 0009-2673  
 DT Journal  
 LA English  
 OS CASREACT 114:229364  
 AB  $\alpha,\omega$ -Diamino acid derivs., and as lysine and ornithine, were  
 synthesized via cobalt-catalyzed amidocarbonylation of  
 $\omega$ -(phthalimido)alkanals in good yield. The phthalimido group was  
 stable to the conditions of amidocarbonylation. The hydroformylation-  
 amidocarbonylation of N-phthaloyl- $\beta,\gamma$ - and N-phthaloyl-  
 $\gamma,\delta$ -unsatd. amines proceeds very nicely to give  
 $\alpha,\omega$ -diamino acids with good selectivity. Selective  
 deprotection of  $\alpha$ -N-acyl- $\omega$ -N-phthaloyl  $\alpha,\omega$ -amino  
 acids was achieved using hydrazine for the N-phthaloyl group and  
 aminoacylase for the N-acetyl group to afford the optically active  
 $\alpha,\omega$ -diamino acid.  
 IT 133787-09-4P  
 RL: SPN (Synthetic preparation); PREP (Preparation)  
 (preparation of)  
 RN 133787-09-4 CAPLUS  
 CN 2H-Isoindole-2-hexanoic acid,  $\alpha$ -(benzoylamino)-1,3-dihydro-1,3-dioxo-  
 , methyl ester (CA INDEX NAME)



L6 ANSWER 21 OF 22 CAPLUS COPYRIGHT 2007 ACS on STN  
 AN 1973:72548 CAPLUS  
 DN 78:72548  
 OREF 78:11545a,11548a  
 TI N-Phthaloylation of chloro- and hydroxy-2-amino acids  
 AU Clarke, S.; Hider, R. C.; John, D. I.  
 CS Dep. Biochem., Yale Univ., New Haven, CT, USA  
 SO Journal of the Chemical Society, Perkin Transactions 1: Organic and  
 Bio-Organic Chemistry (1972-1999) (1973), (3), 230-4  
 CODEN: JCPRB4; ISSN: 0300-922X  
 DT Journal  
 LA English  
 OS CASREACT 78:72548  
 AB N-Phthaloylation of 4-chloro- and 4-hydroxy-2-amino acids was achieved in  
 40-88% yield with N-(ethoxycarbonyl)phthalimide (I) (1.1 equivalent) in Me<sub>2</sub>SO  
 containing Et<sub>3</sub>N; thus prepared were the N-phthaloyl derivs. of  
 Cl(CH<sub>2</sub>)<sub>2</sub>-CH(NH<sub>2</sub>)CO<sub>2</sub>Me (II), the Me esters of 3-chloroalanine, and  
 4-chloronorvaline, and the lactone of 4-hydroxyisoleucine. Phthaloylation of  
 4-chlorolysine Me ester gave 26% of the N<sub>6</sub>-phthaloyl and N,N'-diphthaloyl  
 derivs. Similarly, phthaloylation of the lactone of 4-hydroxylysine gave  
 a mixture of the N<sub>6</sub>-phthaloyl and N,N'-diphthaloyl derivs. The rates of  
 cyclization of the intermediates o-(EtO<sub>2</sub>CNHCO)C<sub>6</sub>H<sub>4</sub>CONHR (R =  
 Cl(CH<sub>2</sub>)<sub>2</sub>-CHCO<sub>2</sub>Me, PhCH<sub>2</sub>, Bu) isolated from the reactions of I with II,  
 PhCH<sub>2</sub>NH<sub>2</sub>, and BuNH<sub>2</sub>, resp., confirmed the mechanism proposed for  
 aminolysis of I.  
 IT 39739-20-3P  
 RL: SPN (Synthetic preparation); PREP (Preparation)  
 (preparation of)  
 RN 39739-20-3 CAPLUS  
 CN 2H-Isoindole-2-hexanoic acid, α-(benzoylamino)-γ-chloro-1,3-  
 dihydro-1,3-dioxo-, methyl ester, [S-(R\*,R\*)]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L6 ANSWER 22 OF 22 CAPLUS COPYRIGHT 2007 ACS on STN  
 AN 1963:33274 CAPLUS  
 DN 58:33274  
 OREF 58:5631d-g  
 TI 1,5,9-Triaminononane derivatives  
 AU Ose, Shinsuke; Takamatsu, Hideji; Saeki, Takeji  
 CS Dai-nippon Pharm. Co., Osaka  
 SO Yakugaku Zasshi (1962), 82, 1197-9  
 CODEN: YKKZAJ; ISSN: 0031-6903  
 DT Journal

LA Unavailable

AB A solution of 21 g. 1,9-dibromo-5-aminononane-HCl in C<sub>6</sub>H<sub>6</sub> is refluxed with 12 g. BzCl 16 hrs. to give 20.1 g. 1,9-dibromo-5-benzamidononane (I), m. 82-3° (ligroine). A solution of I in C<sub>6</sub>H<sub>6</sub> is refluxed with Me<sub>2</sub>NH 15 hrs. to give 1,9-bis(diethylamino)-5-benzamidononane (II), m. 82-3°. Similarly prepared are the following [R(CH<sub>2</sub>)<sub>4</sub>]<sub>2</sub>CHNHBz (R and m.p. given): piperidino, 90-2°; morpholino, 98-101°; pyrrolidino, 89-91°; 1,2,3,4-tetrahydro-2-isoquinolyl, 111-12°; 1,2,3,4-tetrahydro-1-quinolyl, 134-5°. II is heated with 20 times excess H<sub>3</sub>PO<sub>4</sub> at 180-5° 12 hrs. to give 1,9-bis(diethylamino)-5-aminonane (III), sirupy. Similarly are prepared the following [R(CH<sub>2</sub>)<sub>4</sub>]<sub>2</sub>CHNH<sub>2</sub>R (R and b.p./mm. given): piperidino, 186-7°/2; morpholino, 200-4°/3.5; pyrrolidino, 162-3°/1; 1,2,3,4-tetrahydro-2-isoquinolyl, sirupy; 1,2,3,4-tetrahydro-1-quinolyl, sirupy. III is heated with HCHO and HCO<sub>2</sub>H, made alkaline with NaOH, and extracted with Et<sub>2</sub>O to give

1,9-bis(diethylamino)-5-dimethylaminonane (IV), b<sub>1</sub> 118°; trihydrochloride m. 247°. Similarly are prepared the following [R(CH<sub>2</sub>)<sub>4</sub>]<sub>2</sub>CHNMe<sub>2</sub> (R, b.p./mm., and m.p. of trihydrochloride given): piperidino, 177°/1, 256°; morpholino, 185°/2, 254-6°; pyrrolidino, 158-160°/1, 230-1°; 1,2,3,4-tetrahydro-2-isoquinolyl, 250°/0.4, 115-18°. IV is allowed to stand with MeBr in EtOH to give the corresponding methobromide, m. 267-8° (EtOH). Similarly prepared are following [R<sub>2</sub>MeN<sup>+</sup>(CH<sub>2</sub>)<sub>4</sub>]<sub>2</sub>CHN<sup>+</sup> Me<sub>3</sub>.3Br<sup>-</sup> (R<sub>2</sub>N and m.p. given): piperidino, 280-1°; morpholino, 259-60°; pyrrolidino, 277-8°; 1,2,3,4-tetrahydro-2-isoquinolyl, 232-3°; 1,2,3,4-tetrahydro-1-quinolyl, 133-6°.

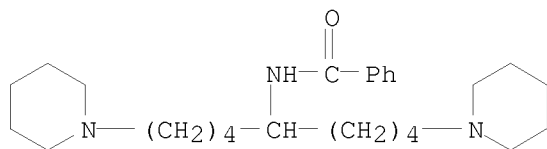
IT 96173-74-9P, Benzamide, N-[5-piperidino-1-(4-piperidinobutyl)pentyl]- 96586-63-9P, Benzamide, N-[5-(1-pyrrolidinyl)-1-[4-(1-pyrrolidinyl)butyl]pentyl]- 97573-27-8P, Benzamide, N-[5-(3,4-dihydro-2(1H)-isoquinolyl)-1-[4-(3,4-dihydro-2(1H)-isoquinolyl)butyl]pentyl]- 97573-28-9P, Benzamide, N-[5-(3,4-dihydro-1(2H)-quinolyl)-1-[4-(3,4-dihydro-1(2H)-quinolyl)butyl]pentyl]-

RL: PREP (Preparation)

(preparation of)

RN 96173-74-9 CAPLUS

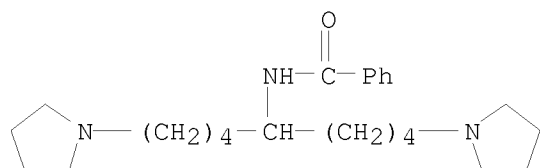
CN Benzamide, N-[5-piperidino-1-(4-piperidinobutyl)pentyl]- (7CI) (CA INDEX NAME)



RN 96586-63-9 CAPLUS

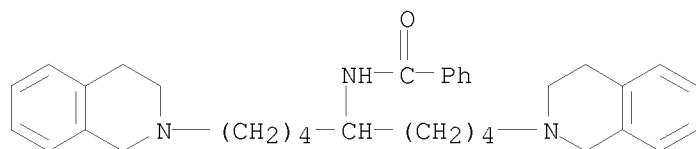
CN Benzamide, N-[5-(1-pyrrolidinyl)-1-[4-(1-pyrrolidinyl)butyl]pentyl]- (CA INDEX NAME)

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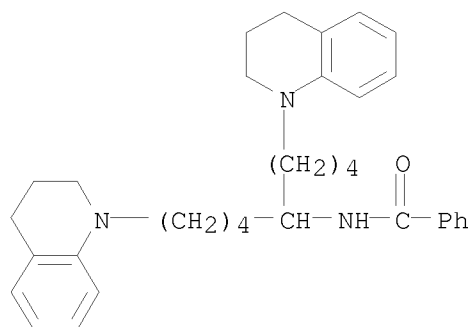
RN 97573-27-8 CAPLUS

CN Benzamide, N-[5-(3,4-dihydro-2(1H)-isoquinolyl)-1-[4-(3,4-dihydro-2(1H)-isoquinolyl)butyl]pentyl]- (7CI) (CA INDEX NAME)



RN 97573-28-9 CAPLUS

CN Benzamide, N-[5-(3,4-dihydro-1(2H)-quinolyl)-1-[4-(3,4-dihydro-1(2H)-quinolyl)butyl]pentyl]- (7CI) (CA INDEX NAME)



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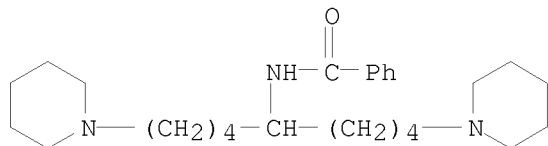
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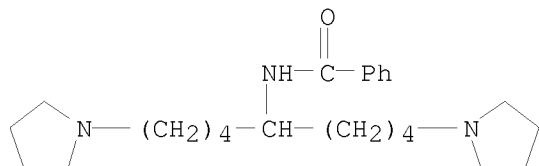
L7 1 L5

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L7 ANSWER 1 OF 1 CAOLD COPYRIGHT 2007 ACS on STN  
 AN CA58:5631d CAOLD  
 TI 1,5,9-triaminononane derivs.  
 AU Ose, Shinsuke; Takamatsu, H.; Saheki, T.  
 TI catalytic dehydrogenation of aldehydecollidine  
 AU Oga, Taijiro  
 IT 96173-74-9 96586-63-9 97573-27-8  
 97573-28-9  
 RN 96173-74-9 CAOLD  
 CN Benzamide, N-[5-piperidino-1-(4-piperidinobutyl)pentyl]- (7CI) (CA INDEX NAME)



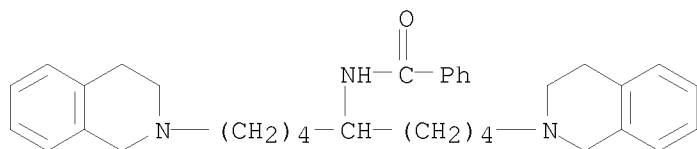
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RN 97573-27-8 CAOLD  
 CN Benzamide, N-[5-(3,4-dihydro-2(1H)-isoquinolyl)-1-[4-(3,4-dihydro-2(1H)-isoquinolyl)butyl]pentyl]- (7CI) (CA INDEX NAME)

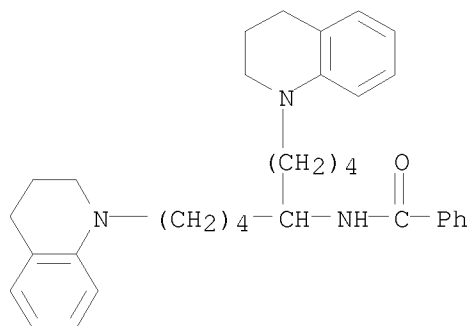


10/539372



RN 97573-28-9 CAOLD

CN Benzamide, N-[5-(3,4-dihydro-1(2H)-quinolyl)-1-[4-(3,4-dihydro-1(2H)-quinolyl)butyl]pentyl]- (7CI) (CA INDEX NAME)



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FULL ESTIMATED COST

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Publication Date (PD): 2 Oct 2007

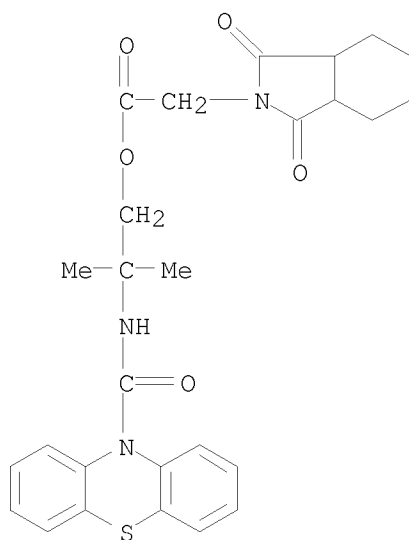
Order Number (ON): 6186-3776

Chemical Name (CN): 2H-Isoindole-2-acetic acid, octahydro-1,3-dioxo-, 2-methyl-2-[(10H-phenothiazin-10-ylcarbonyl)amino]propyl ester

CAS Registry No. (RN): 511513-88-5

Supplementary Term (ST): CHEMICAL LIBRARY

Structure :



L8 ANSWER 2 OF 15 CHEMCATS COPYRIGHT 2007 ACS on STN

Accession No. (AN): 2037170526 CHEMCATS

Catalog Name (CO): New Chemistry Horizons Laboratories Screening Library

Publication Date (PD): 8 Nov 2007

Order Number (ON): NCHSC2-79979

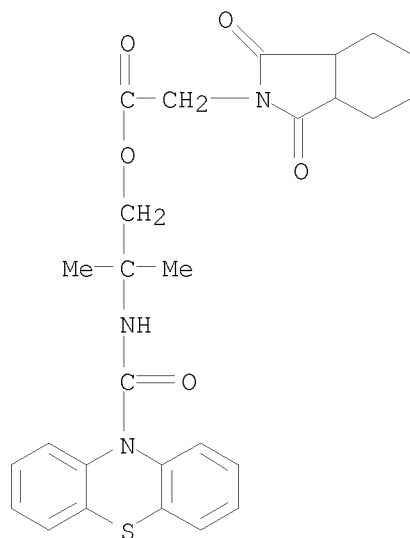
Chemical Name (CN): 2H-Isoindole-2-acetic acid, octahydro-1,3-dioxo-, 2-methyl-2-[(10H-phenothiazin-10-ylcarbonyl)amino]propyl ester

CAS Registry No. (RN): 511513-88-5

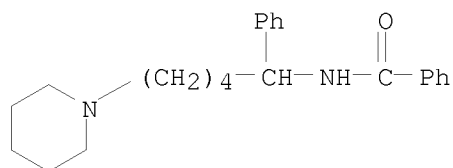
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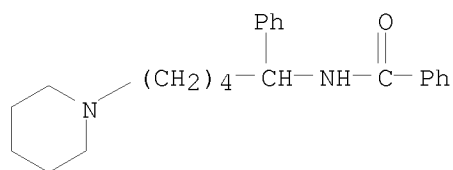


L8 ANSWER 4 OF 15 CHEMCATS COPYRIGHT 2007 ACS on STN  
 Accession No. (AN): 2036286427 CHEMCATS  
 Catalog Name (CO): Ambinter Stock Screening Collection  
 Publication Date (PD): 1 Jun 2007  
 Order Number (ON): STOCK1S-00425  
 Chemical Name (CN): Benzamide, N-[1-phenyl-5-(1-piperidinyl)pentyl]-  
 CAS Registry No. (RN): 171203-85-3  
 Supplementary Term (ST): CHEMICAL LIBRARY  
 Structure :

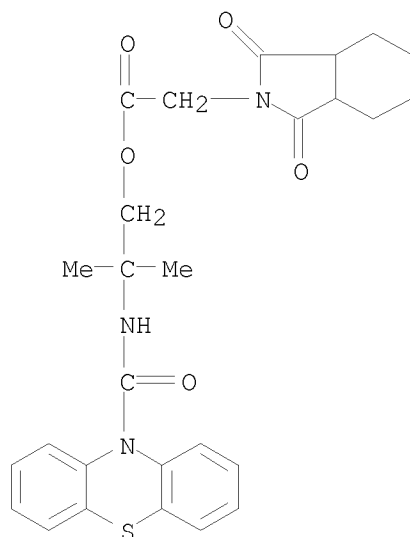


L8 ANSWER 5 OF 15 CHEMCATS COPYRIGHT 2007 ACS on STN  
 Accession No. (AN): 2031192446 CHEMCATS  
 Catalog Name (CO): Aurora Screening Library  
 Publication Date (PD): 6 Sep 2007  
 Order Number (ON): kbs-008261  
 Chemical Name (CN): Benzamide, N-[1-phenyl-5-(1-piperidinyl)pentyl]-  
 CAS Registry No. (RN): 171203-85-3  
 Supplementary Term (ST): CHEMICAL LIBRARY  
 Structure :

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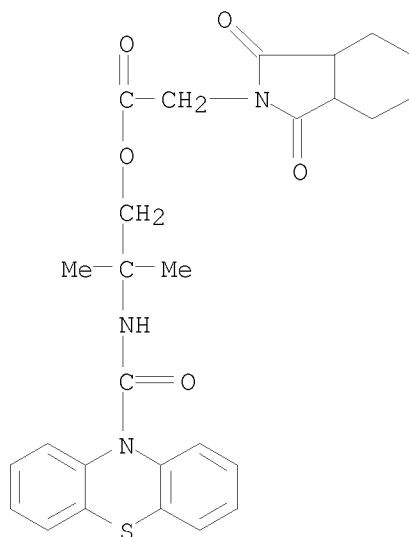
L8 ANSWER 6 OF 15 CHEMCATS COPYRIGHT 2007 ACS on STN  
Accession No. (AN): 2028002259 CHEMCATS  
Catalog Name (CO): MicroChemistry Screening Collection  
Publication Date (PD): 25 Apr 2007  
Order Number (ON): 281369  
Chemical Name (CN): 2H-Isoindole-2-acetic acid, octahydro-1,3-dioxo-,  
2-methyl-2-[(10H-phenothiazin-10-ylcarbonyl)amino]propyl ester  
CAS Registry No. (RN): 511513-88-5  
Supplementary Term (ST): CHEMICAL LIBRARY  
Structure :



L8 ANSWER 7 OF 15 CHEMCATS COPYRIGHT 2007 ACS on STN  
Accession No. (AN): 2027695637 CHEMCATS  
Catalog Name (CO): Princeton Gold Collection I  
Publication Date (PD): 13 Jul 2007  
Order Number (ON): OSSK\_540709  
Chemical Name (CN): 2H-Isoindole-2-acetic acid, octahydro-1,3-dioxo-,  
2-methyl-2-[(10H-phenothiazin-10-ylcarbonyl)amino]propyl ester  
CAS Registry No. (RN): 511513-88-5  
Supplementary Term (ST): CHEMICAL LIBRARY

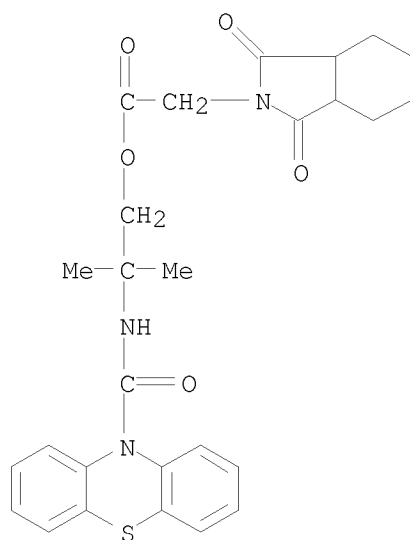
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Structure :

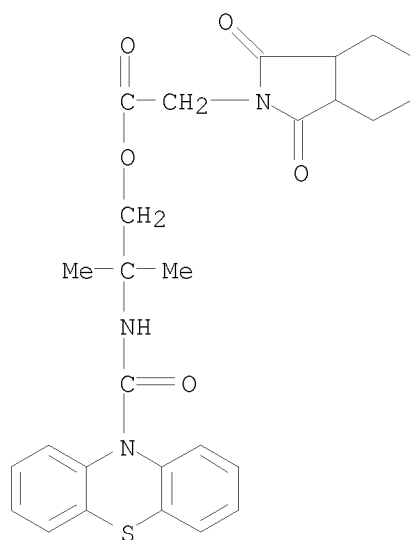


L8 ANSWER 8 OF 15 CHEMCATS COPYRIGHT 2007 ACS on STN  
Accession No. (AN): 2026069766 CHEMCATS  
Catalog Name (CO): Aurora Screening Library  
Publication Date (PD): 6 Sep 2007  
Order Number (ON): kina-0064310  
Chemical Name (CN): 2H-Isoindole-2-acetic acid, octahydro-1,3-dioxo-,  
2-methyl-2-[(10H-phenothiazin-10-ylcarbonyl)aminopropyl ester  
CAS Registry No. (RN): 511513-88-5  
Supplementary Term (ST): CHEMICAL LIBRARY  
Structure :

10/539372



L8 ANSWER 9 OF 15 CHEMCATS COPYRIGHT 2007 ACS on STN  
Accession No. (AN): 2023243378 CHEMCATS  
Catalog Name (CO): Scientific Exchange Product List  
Publication Date (PD): 18 May 2007  
Order Number (ON): M-106500  
Chemical Name (CN): 2H-Isoindole-2-acetic acid, octahydro-1,3-dioxo-,  
2-methyl-2-[(10H-phenothiazin-10-ylcarbonyl)amino]propyl ester  
CAS Registry No. (RN): 511513-88-5  
Supplementary Term (ST): CHEMICAL LIBRARY  
Structure :



L8 ANSWER 10 OF 15 CHEMCATS COPYRIGHT 2007 ACS on STN

Accession No. (AN): 2021307126 CHEMCATS

Catalog Name (CO): AKos Screening Library

Publication Date (PD): 7 Feb 2006

Order Number (ON): AKL-P-1106500

Chemical Name (CN): 2H-Isoindole-2-acetic acid, octahydro-1,3-dioxo-,  
2-methyl-2-[(10H-phenothiazin-10-ylcarbonyl)amino]propyl ester

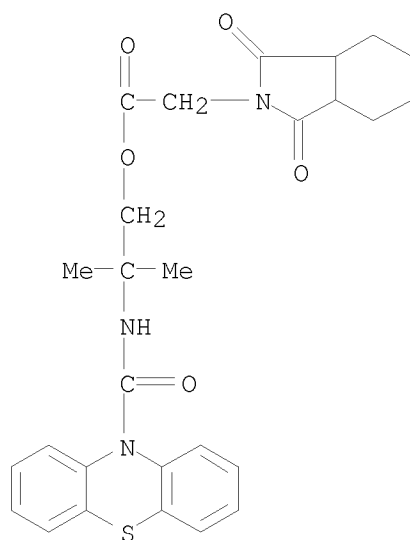
Synonym (CN): Also sold under AKos Order Number(s): STT-00114311,  
OWH-2041105

CAS Registry No. (RN): 511513-88-5

Supplementary Term (ST): CHEMICAL LIBRARY

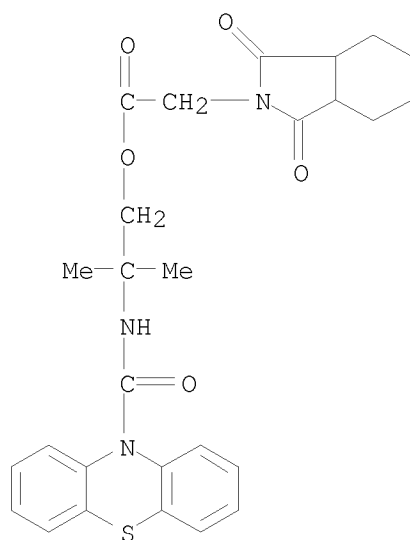
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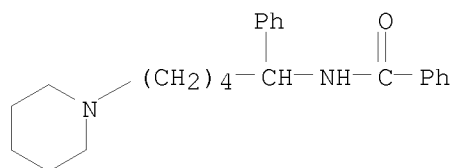


L8 ANSWER 11 OF 15 CHEMCATS COPYRIGHT 2007 ACS on STN

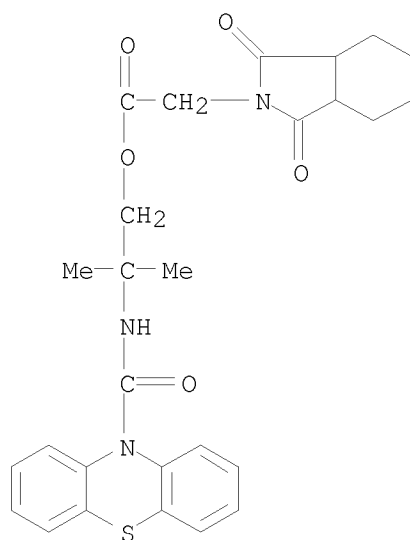
Accession No.	(AN): 2020286708 CHEMCATS
Catalog Name	(CO): Interchim Intermediates
Publication Date	(PD): 9 Jul 2007
Order Number	(ON): STOCK3S-45083
Chemical Name	(CN): 2H-Isoindole-2-acetic acid, octahydro-1,3-dioxo-, 2-methyl-2-[(10H-phenothiazin-10-ylcarbonyl)amino]propyl ester
Synonym	(CN): Also sold under Interchim Order Number(s): AJ-292/41685861, STK135578
CAS Registry No.	(RN): 511513-88-5
Supplementary Term	(ST): CHEMICAL LIBRARY
Structure	:



L8 ANSWER 12 OF 15 CHEMCATS COPYRIGHT 2007 ACS on STN  
 Accession No. (AN): 2020172785 CHEMCATS  
 Catalog Name (CO): Interchim Intermediates  
 Publication Date (PD): 9 Jul 2007  
 Order Number (ON): STOCK1S-00425  
 Chemical Name (CN): Benzamide, N-[1-phenyl-5-(1-piperidinyl)pentyl]-  
 CAS Registry No. (RN): 171203-85-3  
 Supplementary Term (ST): CHEMICAL LIBRARY  
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L8 ANSWER 13 OF 15 CHEMCATS COPYRIGHT 2007 ACS on STN  
 Accession No. (AN): 2017056336 CHEMCATS  
 Catalog Name (CO): Compounds For Screening  
 Publication Date (PD): 6 Nov 2007  
 Order Number (ON): AJ-292/41685861  
 Chemical Name (CN): 2-methyl-2-[(10H-phenothiazin-10-ylcarbonyl)amino]propyl (1,3-dioxooctahydro-2H-isoindol-2-yl)acetate  
 CAS Registry No. (RN): 511513-88-5  
 Supplementary Term (ST): CHEMICAL LIBRARY  
 Structure :



L8 ANSWER 14 OF 15 CHEMCATS COPYRIGHT 2007 ACS on STN

Accession No. (AN): 2014902440 CHEMCATS

Catalog Name (CO): Vitas-M Screening Collection

Publication Date (PD): 7 Jun 2007

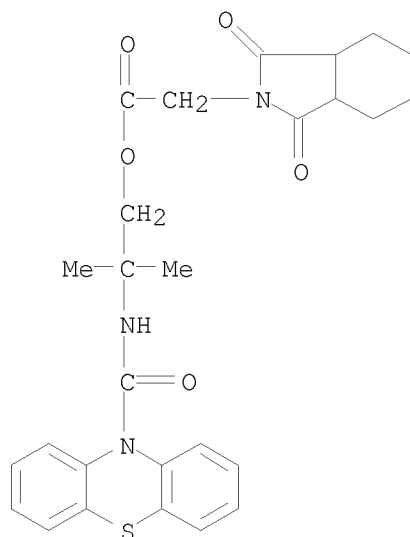
Order Number (ON): STK135578

Chemical Name (CN): 2H-Isoindole-2-acetic acid, octahydro-1,3-dioxo-,  
2-methyl-2-[(10H-phenothiazin-10-ylcarbonyl)amino]propyl ester

CAS Registry No. (RN): 511513-88-5

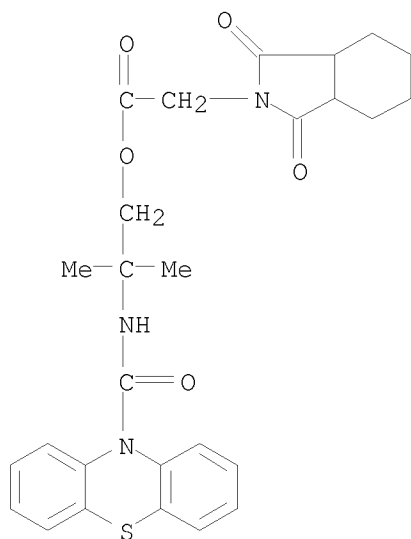
Supplementary Term (ST): CHEMICAL LIBRARY

Structure :



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L8 ANSWER 15 OF 15 CHEMCATS COPYRIGHT 2007 ACS on STN  
Accession No. (AN): 2010420418 CHEMCATS  
Catalog Name (CO): Interbioscreen Compound Library  
Publication Date (PD): 5 Oct 2007  
Order Number (ON): STOCK3S-45083  
Chemical Name (CN): 2H-Isoindole-2-acetic acid, octahydro-1,3-dioxo-,  
2-methyl-2-[(10H-phenothiazin-10-  
ylcarbonyl)aminolpropyl ester  
CAS Registry No. (RN): 511513-88-5  
Supplementary Term (ST): CHEMICAL LIBRARY  
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COST IN U.S. DOLLARS

SINCE FILE	TOTAL
ENTRY	SESSION
30.63	335.70

FULL ESTIMATED COST

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)

SINCE FILE	TOTAL
ENTRY	SESSION
0.00	-17.16

CA SUBSCRIBER PRICE

SESSION WILL BE HELD FOR 120 MINUTES

STN INTERNATIONAL SESSION SUSPENDED AT 12:17:35 ON 27 DEC 2007